Towards Sustainable Development:

Application and Validation of Air Dispersion Model In Urban Environment

Xiangyu Sheng

This thesis is submitted in partial fulfilment of the requirements of the De Montfort University for a degree of

Doctor of Philosophy

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Institute of Energy and Sustainable Development
De Montfort University

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LIST OF SYMBOLS

$\overline{C}_m$	Modelled observed concentrations
$\overline{C}_o$	Observed concentrations respectively, over-bar indicating the averaging procedure with respect to the sampling points
Ki	Ratios $K_i = \overline{C}_{mi}/\overline{C}_{oi}$
Si	Ratios $S_i = \overline{C}_{oi}/\overline{C}_o$
i	i-th receptor
U	Wind speed
U_g	Geostrophic wind speed normalised by the friction velocity
ϕ	Wind direction (angle wind is coming from in degrees clockwise from north, e.g. 180' is a southerly wind
$\Delta\phi$	Geostrophic wind direction minus surface wind direction (degrees)
$F_{\theta 0}$	Surface heat flux (in ADMS output)
$1/L_{mo}$	Reciprocal of the Monin-Obukhov length

$$L_{mo} = \frac{-U_*^3}{\kappa g F_{\theta 0}/(\delta C_p T_0)}$$

Where k is von Karman's constant (=0.4), δ density and C_p specific heat capacity.

h	Boundary layer depth
N_u	Buoyancy frequency above the boundary layer
$\Delta\theta$	Temperature jump across the boundary layer top
T^c_0	Near surface temperature (^{0}C)
P	Precipitation rate (mm/hour)
C_l	Amount of cloud cover (oktas)
r	Surface albedo
α	Modified Priestly-Taylor parameter (as defined in Holtslag and van

	ulden, 1983)
t_{day}	Julian day number
t_{hour}	Local time (hours)
f_r	Frequency of occasions when these conditions occur (arbitrary units, e.g. percentage of occasions or number of hours per year).
σ_θ	Standard deviation of mean wind direction (degrees)
u_*	Friction velocity
U_g	Geostrophic wind speed
U_{g*}	Geostrophic wind speed normalised by the friction velocity
ϕ_0	Surface wind direction (angle wind is coming from in degrees clockwise from north, e.g. 180 is a southerly wind)
ϕ_g	Geostrophic wind direction (angle wind is coming from in degrees clockwise from north)
$\Delta\phi$	Geostrophic wind direction minus surface wind direction (degrees)
w_*	Convective velocity scale if $F_{\theta_0} > 0$, $w_* = (gF_{\theta_0} h / \rho c_p T_0)^{1/3}$; if $F_{\theta_0} \leq 0, w_* = 0$.
F_{θ_0}	Surface heat flux
H	Boundary layer depth
N_u	Buoyancy frequency above the boundary layer
$\Delta\theta$	Temperature jump across the boundary layer top
T_0	Near surface temperature (K)
P	Precipitation rate (mm/hour); P may be missing if insufficient input data are given.
F_r	Frequency of occasions when these conditions occur (arbitrary units, e.g. percentage of occasions or number of hours per year)
σ_θ	Standard deviation of mean wind direction (degree).
$u(z), du/dz, d^2u/dz^2$	Mean wind, velocity and gradients

$\sigma_u(z)$, $\sigma_v(z)$, $\sigma_w(z)$	r.m.s. turbulent velocities
$\Lambda_v(z)$, $\Lambda_w(z)$	Turbulent length scales
$\varepsilon(z)$	Energy dissipation rate
$T_L(z)$	Langrangian time scale
$N(z)$	Buoyancy frequency
$T(z)$	Temperature
$\rho(z)$	Density
Q_s	Emission rate
$h\nu$	Sun Light
ROC	Reactive Organic Compounds
RP	Radical Pool
SGN	Stable Gaseous Nitrogen products
SNGN	Stable Non-Gaseous Nitrogen products
C(t)	Concentration of the chemical species at time t
H_{mix}	Depth of the atmospheric boundary layer
V_d	Applied deposition velocity
F_e	Emission flux of the species
Δt	A time period
$\theta(z)$	Mean potential temperature at height
ρ	Air density
C_p	Specific heat capacity of air
κ	Von Karman's constant (~0-4)
$U(z)$	Mean wind speed at height z
H	Heat flux
Z	Height of measurements (metres)

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DECLARATION

I hereby declare that the following thesis is my own composition, that the work has been carried out by myself and that it has not been presented in any previous application for a higher degree.

Xiangyu Sheng

ABSTRACT

In the new regime of air quality management established by the UK Environment Act, monitoring will continue to provide a basis for assessing urban air quality. However it is not possible, practically or economically, to monitor at every location of interest or predict future levels using this approach alone. In order to achieve estimates of air quality, on both wider spatial and temporal scales, the use of air quality dispersion modelling is becoming more important.

The aim of this project is to evaluate the applicability of the ADMS_Urban air dispersion model to predict pollution levels for the purpose of air quality management. In this study, urban air quality management is reviewed, and a mathematical description of various air dispersion models is presented.

Guidelines for the creation and the application of emission inventory for air dispersion modelling are presented. Air quality patterns and distribution characteristics in the urban area were analysed and evidence for import of key pollutants is presented. This study then focuses on the air dispersion model ADMS_Urban, and its application in Leicester. Performance of the ADMS_Urban model is accessed by comparing predicted levels of pollutants with measurements over a range of time-scales. This study is concerned primarily with the pollutants associated with traffic flows which are the key concerns for Leicester. The strengths and weaknesses and the absolute accuracy of the ADMS_Urban model are discussed. The effectiveness of techniques to model pollutant import and pollutant chemical reactions is assessed. Strategic modelling of pollution levels in Leicester for the year 2005 is presented.

Dedicated to the Memory of Professor Neil T. Bowman

Director of the Institute of Energy and Sustainable Development

1994-1999

CHAPTER 1 INTRODUCTION

PREAMBLE

Population, economic development, natural resources and the state of the environment all play important roles in achieving sustainable development. Of the indicators on the state of the environment, air quality is one of the most important, especially in urban and industrial regions.

Air quality is a significant public concern (DoE, 1995). Air pollution arises from human activities and in particular from industry, transport and both the domestic and commercial sectors. The emissions are diluted and dispersed due to the natural cleansing properties of the atmosphere. Where the input to the atmosphere exceeds the cleansing capacity, then a build up of pollutants may occur. Contemporary air pollution problems, for example those arising from increasing vehicle emissions, have entered the political arena both in Europe and world-wide.

Urban air quality has received much attention in recent years due to the increasing number of health complaints and illnesses related to air pollution has been reported (COMEAP, 1998). There is an increasing understanding of the health effects of current air pollution concentrations. Although there are substantially lower concentrations of visible pollution than in the 1950s (when substantial numbers of people died or suffered ill health in severe episodes of air pollution), there are associations with premature mortality, chronic illness and discomfort for sensitive groups. Again the Department of Health report

(COMEAP, 1998) estimated that up to 24,000 people may die prematurely every year as a result of air pollution. However, air quality is not just an issue of human health. Air pollution can degrade both the natural and man-made environment, including forests, lakes, crops, wildlife and buildings.

Maintenance of and improvements to air quality are central to sustainability. Agenda 21, the central concept to come out of the Rio Earth Summit in 1992, dedicates one of its chapters to "protecting and promoting human health" (DoE, 1997). Air quality is defined as a key element in the reduction of health risks from environmental pollution. This has also been reflected in the UK's Sustainable Development Strategy (DoE, 1994). In acknowledging that good air quality is essential for human health and the well-being of the environment as a whole, it identified one of the key issues for sustainability as to "manage local air quality, especially in urban areas, and in particular to ensure that all relevant sectors - industry, transport, local authorities and the general public contribute" (DoE, 1997).

Emissions of pollutants and other products of combustion are a key indication of the state of the environment in any location. Thus assessment and subsequent management of emissions contribute to the quality of the environment and sustainable development. In this chapter legislation currently enacted to limit pollutant emissions and hence improve air quality and methods by which air quality may be assessed are reviewed.

1.1 AIR POLLUTION ABATEMENT

The damages caused by air pollution in Europe are large and it is generally accepted that there is an urgent need for reduced emissions to the atmosphere (WHO, 1995). The damages are caused by high ambient air concentrations and depositions of many chemical components. Among the most important components are acidifying constituents (sulphur and both oxidised and reduced nitrogen compounds), photochemical components (including Ozone), particulate matters and toxic compounds such as metals, organic compounds and others. The concentrations and depositions are dependent on

- The total mass of pollutants emitted to the atmosphere and its spatial and temporal distribution.
- Transport and transformation processes in the atmosphere.
- Deposition processes.

Assessments of emission reduction strategies must consider all three factors and the complexity of these problems necessitates the use of atmospheric models. Average exposure of the ecosystem to concentrations and deposition, emission scenario studies and linkage to economical aspects and cost effectiveness are all examples of areas where the models are needed.

The development of emission reduction strategies for acidifying components in Europe under the United Nations Economic Commission for Europe (UN-ECE) Convention and the Convention on Long Range Transboundary Air Pollution is a good example of how models can play an important role in the decision making process toward protocols on emission reductions. Regional scale models, quantifying the transboundary

fluxes of air pollution between the European countries and deposition to ecosystems, have been applied together with knowledge on ecosystem critical loads of acidity and the costs involved in emission reduction in order to find optimal solution for the reductions (Barrett et al., 1995). This led to a renewal of the second sulphur protocol in 1994 aiming at further substantial reductions in SO_2 emissions by 2010. In further work on new protocols on reduction of nitrogen emissions and emissions of volatile organic compounds (VOC), atmospheric models will have to play an even more important role due to increased complexity of the problems. Further linkage of local to regional scale and regional to global scale air pollution problems will require an intensified usage of models.

1.2 AN OVERVIEW OF URBAN AIR QUALITY MANAGEMENT

1.2.1 Legislation Background

Legislation exists throughout most of the world to limit both pollutant emissions and concentrations in the air. The tightest standards currently under consideration are those of the European Union (EU) which has been legislating to control emissions of air pollutants and to establish environmental quality objectives for the last two decades. These cover environmental quality standards, vehicle emission standards, fuel quality standards, industry pollution control and environmental impact assessment. Most recently, the European Commission (EC) Council of Ministers has adopted two directives central to European air and pollution policy.

The Ambient Air Quality Assessment and Management Directive (1996) establishes a framework under which the Community will agree air quality limit or guide values for specified pollutants in a series of ' sub-directives'.

The Integrated Pollution Prevention and Control Directive (1996) will be the cornerstone of European industrial pollution control policy. It is a source-based Directive, requiring Member States to ensure that major industrial installations receive permits based on the Best Available Techniques for pollution control, subject to technical and economic feasibility, taking into account discharges to all environmental media.

Historically, the control of air pollution has developed on a reactive basis, with regulations to address specific problems as they became evident. For example, the Clean Air Acts (UK 1956 and 1968) tackled the problem of black smoke, and to a lesser extent, sulphur dioxide from both domestic and industrial sources. By introducing smoke control areas, urban air quality was greatly improved.

The Environmental Protection Act 1990 focussed on industrial sources of air pollution. It described two lists, 'Part A' and 'Part B' processes for which authorisations were required due to the potential for emissions to air, water or land. The complex and large-scale 'Part A' processes were under the control of Her Majesty's Inspectorate of Pollution (which in April 1996 became the Environment Agency and its Scottish and Northern Ireland counterparts). The emissions to air from more numerous 'Part B' processes are the responsibility of local authorities (environmental health departments). The Act also requires environmental information relating to the application, authorisation and subsequent emissions data to be made available through public registers.

The impetus for change has been the gradual recognition that policies and tools developed for the reduction of visible air pollution are no longer appropriate for the management of air quality. Whilst the UK can rightly claim successful previous implementation of policy in regard to smoke pollution, it is no longer an appropriate policy response for contemporary problems. Regions now confront quite different air pollution problems when compared to the situation 30 years ago. Contemporary problems are associated with the emissions of a variety of primary pollutants, with numerous and varied sources, many of which undergo subsequent chemical transformations into secondary pollutants. Hence, a new policy framework was required with a new approach to the more complex air quality situation. The Environment Act 1995 (Part IV) introduced a more holistic approach. It required the Secretary of State to prepare and publish a strategic framework for the management of national air quality. This was published as the National Air Quality Strategy (NAQS) (DOE, 1997) which outlined a comprehensive approach to control emissions from main sources and to improve ambient air quality through a nation-wide system of local air quality management, as well as through national policy instruments. This policy response was explicitly concerned with the impact of air pollution on human health.

In common with sustainable development goals, the responsibility for reaching certain standards and objectives for the eight pollutants addressed by the NAQS fell mainly on local authorities. The Air Quality Regulations 1997 gave legal weight to standards and objectives for eight pollutants, seven of which require local authorities to take local air quality management action through specific objectives.

The National Air Quality Strategy assigns air quality objectives to be met by the end of 2005 (DoE, 1997) as follows in Table 1.1.

Table 1.1 National Air Quality Standards and Specific Objectives (source: DoE, 1997)

Pollutant	Standard Concentration	Measured as	Specific Objective
Benzene	5 ppb	running annual mean	achieve by 2005
1,3 Butadiene	1 ppb	running annual mean	achieve by 2005
Carbon monoxide	10 ppm	running 8-hour mean	achieve by 2005
Lead	0.5 $\mu g/m^3$	annual mean	achieve by 2005
Nitrogen dioxide	150 ppb	1 hour mean	99.9th percentile by 2005*
	21 ppb	annual mean	achieve by 2005*
Ozone	50 ppb	running 8-hour mean	97th percentile by 2005*
Particles PM_{10}	50 $\mu g/m^3$	Running 24-hour mean	99th percentile by 2005*
Sulphur dioxide	100 ppb	15-minute mean	99.9th percentile by 2005*

*provisional objectives - all to be reviewed by 2000. The percentiles mean that: Nitrogen dioxide - 8 hours exceedence per year allowed; Ozone target to be achieved on all but 10 days per year; Particles target to be achieved on all but 4 days per year; Sulphur dioxide - 99.9% of measurements to be below 100 ppb.

The averaging periods reflect the nature of potential health effects. Pollutants with shorter averaging periods having an acute health effect and those with longer averaging periods representing a chronic health effect.

Part IV of the Environment Act requires a review and assessment of air quality as the first step in the local air quality management regime. The government has recommended a 3-stage approach, whereby each stage increases in detail and complexity. The complexity and detail of the review and assessment should be consistent with the risk of failing to

achieve the air quality objectives by the end of 2005. On completion of a third stage, in areas where it appears that the objectives are likely to be breached by the end of 2005, an Air Quality Management Area (AQMA) must be designated. Where AQMAs have been designated, local authorities are required to prepare a written air quality action plan setting out how the authority will attempt to achieve air quality standards and objectives in the designated area (DETR, 1997a-h).

The UK is also required to implement European Union directives. The Ambient Air Quality Directive (96/62/EC) provides member states with a basis for local air quality management. Daughter directives will set new standards for specified pollutants. The first daughter directive covering sulphur dioxide (SO_2), nitrogen dioxide (NO_2), particulates (PM_{10}) and lead have now reached a common position and are expected to be enacted imminently. The next daughter directive will cover carbon monoxide and benzene. The UK Government believes that the National Air Quality Strategy will provide the principal means of carrying out its commitments under the EU framework. Due to the faster pace at which the early stages of the NAQS are being implemented in comparison with the EU framework, the UK's experience is providing useful insight for other Member States faced with implementing the EC framework (Elsom, 1999).

1.2.2 UK National Air Quality Strategy

Key Elements of the Strategy

The Strategy sets out a national framework for reducing hazards to health from air pollution in the UK. It identifies air quality standards for eight priority pollutants based upon the recommendations of the Government's Expert Panel on Air Quality Standards

(EPAQS) where available, or World Health Organisation guidance where no EPAQS recommendation exists. Objectives for improving ambient air quality set out the degree of compliance with each standard to be achieved by the year 2005 (Table 1.1).

Meeting Targets

It is acknowledged that objectives for nitrogen dioxide, particulates, ozone and sulphur dioxide are unlikely to be met in some parts of the UK unless further action is taken (DoE, 1997). The transport sector, local authorities and industry are identified as key contributors to meeting the Strategy's aims. A National Air Quality Forum has been formed to review trends in air quality and implementation of the Strategy. It comprises representatives of industry, central and local government, business and Non-Governmental Organisations (NGOs).

Local Air Quality Management (LAQM)

The Strategy acknowledges that current national policies, combined with the tighter vehicle emission standards agreed by the EU, will not be enough to meet air quality standards across the country by 2005. Local authority action will be required to "mop up" the remaining pollution hotspots. The specific objectives will form the basis for the designation of air quality management areas (AQMAs) under the Environment Act 1995, with the exception of ozone, which is not easily controlled by local measures.

The regulations enforcing AQMA were implemented in December 1997. Implementation of the Strategy involves two stages. Firstly all local authorities must review and assess air quality by December 1999. If this stage suggests that air quality objectives will not be met, they will have to declare AQMAs and put together action plans to show

how these standards can be met by 2005. In undertaking these duties, Local Authorities (LAs) must have regard to guidance issued by DoE. As well as reviewing air quality, the Strategy states that all authorities should develop a Local Air Quality Strategy (LAQS) to ensure that air quality is integrated into planning and transport policy. The LAQS might cover co-operation within and between LAs; involving and informing business and the community; local statutory and voluntary measures.

Implications for Local Authorities (LAs)

All Local Authorities (LAs) will need to act on review and Local Air Quality Strategy (LAQS). Concerns will include:

Responsibility - Air pollution is traditionally an environmental health function. The new air quality managers will have to make stronger links with planners, engineers and environment policy officers.

Resources - Experience from the first phase will provide further information about the resource implications of LAQM, but the demand is likely to be for specialist staff time rather than new equipment.

Consensus - Some LAQM measures could prove controversial. LAs need to inform the public and local business about air quality and involve them in reaching consensus on the LAQS.

Business and Industry

The Strategy says that in principle, reductions in emissions will be sought where they are most cost effective, both within and between industrial sectors. For industrial processes regulated for Integrated Pollution Control (IPC) or Local Air Pollution Control

(LAPC) under the Environmental Protection Act, the regulators (Environmental Agency or LAs) may seek to impose tighter standards than might otherwise be justified if industry is a significant contributor to local air pollution. Other industries and businesses face the prospect of new controls on small combustion plant, as well as encouragement to participate in a wider range of energy and environmental management schemes. VOC emissions will also be targeted.

1.3 THE MAJOR POLLUTANTS

This section introduces the characters of major pollutants and their health effects to human being.

Benzene

Benzene is a known human carcinogen. Occupational exposure to benzene at 1-10 ppm is strongly linked with the risk of developing leukaemia (also less strongly with liver, lung and stomach cancer) (EPAQS, 1994a).

1,3-Butadiene

1,3-Butadiene is an accepted genotoxic carcinogen and therefore no absolutely safe concentration can be defined. Laboratory studies have shown that 1,3-butadiene causes a variety of cancers in rodents and damages the genetic structures of the cell (EPAQS, 1994b).

Carbon monoxide

Carbon monoxide diminishes the oxygen carrying capacity of the blood by binding to haemoglobin. In low concentrations (2-3%), it causes headaches, impaired concentration

and impaired reflexes. Low concentrations can also increase the risk of heart problems in individuals with cardiovascular disease. Mental activity may also be affected by reductions in oxygen supply resulting from exposure to carbon monoxide. For example, such changes may affect hand-eye co-ordination. Other concerns include the risk to pregnant women from exposure to high levels of carbon monoxide, which can cause foetal growth retardation (EPAQS, 1994c).

Lead

Lead exhibits toxic biochemical effects in humans, which lead to a decrease in the synthesis of haemoglobin, acute or chronic damage to the nervous system and effects on the kidneys, gastrointestinal tract, joints and reproductive system. Anaemia only occurs in cases of severe lead poisoning, but effects on red cell survival and haemoglobin production are found at lower concentrations (EPAQS, 1998).

Nitrogen dioxide

Nitrogen dioxide can affect lung function. Repetitive exposure in animals can produce changes in lung structure, lung metabolism, and lung defences against bacterial infection. Animal toxicological studies suggest that peak concentrations contribute more to the toxicity than does the duration of the exposure, although the latter is still important. This is the reason for having two objectives, both hourly means and an annual mean. There is also some evidence to support that exposure to nitrogen dioxide may put children at an increased risk of respiratory infection and may lead to impaired lung function later in life (EPAQS, 1996).

Particulates (PM_{10})

Particulate matter with a diameter of less than 10 μm is known as PM_{10}. It is this size range of particulate matter suspended in air that has been found to have human health effects. It is implicated in increasing obstruction of the airways and worsening underlying lung disease. There is also a possibility that some particulates penetrate deep into the lung tissue and may be carcinogenic (for example, these particles that contain hydrocarbons). Although many of the obvious effects of air pollution disappeared with the earlier smog, research over the last few years has suggested that, even at much lower levels now found in the UK, particulate air pollution seems to be associated with a range of measures of ill health, including effects on cardiovascular and lung function and asthma (EPAQS, 1995a).

Sulphur dioxide

Sulphur dioxide and its associates are the main cause of acid rain. Sulphur dioxide is a potent bronchorestricting agent. The degree of effect depends on the concentration inhaled, degree of underlying airway reactivity, the rate of exercise of the individual, the amount of moisture in the inhaled air and the distribution of inhaled air between the nose (effective filter) and the mouth (poor filter) (EPAQS, 1995b).

Ozone

Ozone is the major indictor of the presence of urban photochemical smog. Short-term health effects include pulmonary function changes, increased airway responsiveness to broncho-constrictors, and airway inflammation. There is also evidence that ozone can cause airway changes that increase the sensitivity of subjects to inhaled allergens such as pollen (EPAQS, 1994d).

1.4 THE SOURCES OF URBAN AIR POLLUTION

There are two main sources of air pollution: industry and transport.

1.4.1 Air Pollution from Industry and Transport

Air pollution in the UK has traditionally been associated with industrial activity and with the domestic burning of coal. These remain important. However, in recent decades, transport emissions have grown to match or exceed other forms of pollution. In urban areas, they have become the dominant source of air pollution emissions (Banister and Button, 1993).

Between 1984 and 1994 the number of cars increased from just over 16 million to about 20.5 million in the UK. The distance they travelled increased significantly and is projected to continue growing (DoE, 1994). Until the 1980s, the increase in road transport was accompanied by a similar increase in the main air pollutants. However, the introduction and promotion of unleaded fuel and tighter vehicle standards, in particular the introduction of catalysts, are reversing this trend. As cleaner vehicles enter the market place over the next decade, these improvements should outweigh the effect of continued growth (DoE, 1995).

Table 1.2 shows the proportions of national emissions attributable to industry and transport. Industry sources are the dominant source of some pollutants, such as sulphur dioxide; significant contributors of others, such as VOCs and lead; and less significant emitters of carbon monoxide, which is generated mainly from traffic. Emissions from road transport, account roughly for the emissions also shown in Table 1.2.

Table 1.2 Industry and Transport Emissions in the United Kingdom

(Data Sources: DoE, 1997)

Pollutant (Kilotonnes)	1996 National Emissions	Industry % of national emissions	Road transport % of national emissions
Benzene	42	32	64
1,3 – Butadiene	10.6	18	68
CO	5475	3	71
Lead	1.399	31	61
NO_x	2018	38	48
PM_{10}	207	56	23
SO_2	2025	90	2

1.4.2 Sources of the Pollutants

According to the publications of the Department of Environment (DoE, 1997), the source of the different pollutants is as summarised below.

Benzene

In the UK the main atmospheric source of benzene is the combustion and distribution of petrol, of which it is a minor constituent (2% by volume). Motor vehicles are the most important single source on a national basis. In 1996 they accounted for 64% of the total UK annual emission of 42 kilotonnes, with most of this arising from petrol vehicles. 32% of the total emissions, were emitted from industrial processes, for example petrochemical processors.

1,3-Butadiene

1,3-Butadiene in the atmosphere is mainly derived from the combustion of petrol and other materials. Although neither petrol nor diesel fuel contains 1,3-butadiene it is formed in the combustion process from olefins in the fuel. 1,3-Butadiene is also an important industrial chemical and is handled in bulk at a small number of locations, for example for use in rubber processes. Other than these locations, the dominant source of 1,3-butadiene in the UK atmosphere is the motor vehicle.

Carbon monoxide

The main source of carbon monoxide in the UK is road transport, which accounted for 71% of the total emission of 5.5 million tonnes in 1996. Road transport sources constitute the larger proportion of all sources in most cities, and maximum 8-hour concentrations are therefore expected near busy and especially congested roads.

Lead

Lead is the most widely used non-ferrous metal and has a large number of industrial applications, both in its elemental form and in alloys and compounds. The single largest use globally is in the manufacture of batteries. Other uses of lead are in paints, glazes, alloys, radiation shielding, tank lining and piping. The compound tetraethyl lead has been used as a petrol additive to enhance the octane rating. However, this use is declining rapidly with the recognition of the adverse effects of lead on human health and the growing use of catalytic converters, which cannot be used with leaded petrol. Most of the current emissions of lead in the UK arise from leaded petrol fuelled motor vehicles. However, leaded petrol will be withdrawn from sale in UK by 1 January 2000.

Nitrogen dioxide

Nitrogen dioxide (NO_2) and nitric oxide (NO) are both oxides of nitrogen and together are referred to as NO_x. All combustion processes produce some NO_x, but the main sources of NO_x in the UK are road transport (48% in 1996), industry (38% in 1996). In urban areas, the proportion of local emissions due to road transport is higher than that in rural areas.

NO_2 is produced by the oxidation of NO in the atmosphere and there is a complex relationship between emissions of NO_x and the resulting concentrations of NO_2, dependent on the proportion of NO_2 in the primary emission and the availability of atmospheric oxidant, especially ozone, to oxidise NO to NO_2.

Particulates (PM_{10})

Unlike the gaseous pollutants discussed in this chapter, which are single, well-defined substances, particulate matter in the atmosphere is composed of a wide range of materials arising from a variety of sources. During 1996, 23% of UK emissions of primary PM_{10} was derived from road transport sources, 56% from industrial sources and power stations. In general, emission estimates for PM_{10} are less accurate than for the other pollutants described above, particularly for sources other than road transport.

Over the last two years, a growing body of evidence has suggested that remote pollution sources play a major role in determining PM_{10} concentrations, even in urban areas. A report by the Airborne Particles Expert Group (APEG, 1999) confirms that long-range transport of secondary particles from Europe and elsewhere in the UK can dominate

the exceedences of the standard for PM_{10}. Secondary pollutants are formed in the atmosphere from emissions of SO_2 and NO_x.

Sulphur dioxide

Sulphur dioxide is emitted through the combustion of coal and oil. The main sources in 1996 were power generation (65%), other industry (24%), commercial and domestic heating (6%) and road transport (2%). Exceedences of the air quality standard currently occur in the vicinity of industrial processes for which stack heights were designed to meet earlier less rigorous air quality standards and in areas where significant quantities of coal are used for space heating.

Ozone

Ozone is not emitted directly from any man-made source in significant quantities, but arises from chemical reactions in the atmosphere. It is primarily formed by a complicated series of chemical reactions initiated by sunlight. Oxides of nitrogen (NOx) and hydrocarbons, derived mainly from man-made sources, react to form ozone. These substances are produced by combustion and other industrial processes. Although NO_x and hydrocarbons are the most important precursors of elevated levels of ozone, production of ozone can also be stimulated by carbon monoxide or methane.

1.4.3 A Strategy for Transport and Air Quality

As transport is one of the most significant factors affecting urban air quality, in "Air Quality: Meeting the Challenge" (DoE, 1995), the UK government set out key principles that it would follow to secure reductions in air pollution:

- improvements in vehicle and fuel technology to reduce emissions;

- tighter controls on the existing vehicle fleet, its management and operation;
- development of environmental responsibilities by fleet operators, and by the public at large, in transport and vehicle use; and
- changes in planning and transport policies which would reduce the need to travel and the reliance on the car.

It is the Government's view that an effective strategic policy must incorporate all these four elements. At the heart of the policy is the need to balance them in the most cost-effective manner. It must be recognised however that they operate over different time scales. It requires time for changes in vehicle technology to be applied, normally at least five years, although changes may in some cases be achievable over a shorter time scale. Changes within the planning systems can take even longer to show significant results and it may only be some years into the next century that current changes in policy will have effect. For short term improvement, it is necessary to look at vehicle inspection and maintenance, at traffic management practices and transport systems, and at driving behaviour.

Given these differences in time scale, practicality and cost effectiveness, the Government proposes that the central elements of its strategy for transport emissions should operate as follows (DoE, 1995):

- the main contribution to securing the necessary reduction in polluting emissions will come from improvements in vehicle technology and fuels. The Government looks to achieve significant reductions in NO_x, PM_{10} and VOCs as a result of the Auto Oil 2000 European standards, and in line with the general principle of cost effectiveness;
- action will also be taken to encourage the use of less polluting alternative fuels, particularly in urban areas;

- in the long term, planning and other measures will help to reduce the need to travel and the reliance on the car. This should help avoid the prospects of an upturn in emissions that might occur from about 2010.

1.5 METHODS AND OBJECTIVES OF THIS STUDY

1.5.1 Methods of Assessing Air Quality

In air pollution assessments, information on all parts of the cause-effect chain should be collected. A physical or chemical description of ambient air not only needs to be presented in a way that it can be compared with effect threshold values (the values which have harmful health effects), but also the relation between this effect quantity and the atmospheric emissions from sources (e.g. source categories, countries, regions, economical sectors) should be quantified (DoE, 1995). When all three elements, (threshold or critical values, ambient parameters and emissions) are available, strategies can be developed. Three types of instruments are used in assessment studies: emission inventories, atmospheric dispersion models and air quality measuring programmes.

Air quality monitoring may be defined as the systematic collection of information from measurements or other means to determine the levels and the time evolution of quantities relevant for air quality (DETR, 1997a). Such quantities are air concentrations, fluxes of air pollutants to land or water surfaces and the exposure to air pollution of human beings, materials and ecosystems.

The aim of air quality monitoring is to get an estimate of the quantities (concentrations, deposition fluxes or exposure) sufficiently representative in time and space

and with the specified accuracy (DETR, 1997e). Spatial scales may range from the very local scale (e.g. street level, direct surroundings of a chimney) to the global scale; time scale may range from minutes (estimation of peak concentrations) up to decades (estimation of trends).

Although measurements form an important aspect of monitoring, measurements alone are rarely sufficient to arrive at the best possible description of the desired concentration. Models are often needed to establish larger scale average exposure that can not easily be derived from measurements (DETR, 1997g). The reason is simply that observations are made at only a few locations and may therefore not be representative of larger areas. Substantial uncertainty can be introduced if measured data are extrapolated or interpolated into large domains and models are therefore used to generate best estimates in situations where measurements are lacking or cannot be made (Elsom, 1999). Models are also necessary if the relative impact of various sources (source categories, emissions from different regions or countries) or emission scenarios have to be investigated.

Atmospheric dispersion models are, generally speaking, any mathematical procedure which produce an estimation of ambient air quality entities (i.e. concentrations, deposition, exceedences) (Finzi et.al, 1982). Dispersion modelling is a key factor in air quality management. Dispersion models are mathematical procedures to describe how pollutants are spread and mixed in the atmosphere (DETR, 1997g). They are often computer based, but simpler nomogram methods (chart or diagram of scaled lines or curves for facilitating calculations) can also be based on physical principles.

Dispersion models are used to assess concentrations of material in the air, for giving advice and for forecasting in emergency or pollution episode situations. In the context of air quality management, it provides a way to calculate the contributions to air quality at a place from the different types of emission sources (DETR, 1997f). This allows the air pollution due to each sector to be reviewed and assessed on a fair basis. Dispersion modelling is also used as a tool to assist decision making and planning. For example, using an air dispersion models to test the air quality impacts of the usage of renewable energy schemes. It could also be used to model pollution scenarios for traffic planning proposals, e.g. clean fuel, electric cars, car parks. Modelling can indicate whether the objectives in the UK Air Quality Strategy are likely to be achieved by the year 2005 (DETR, 1999), and reveal the likely geographical extent of any air pollution "hotspots".

1.5.2 Objectives of the Study

Air quality monitoring will continue to provide a basis for assessing urban air quality, but it is not possible practically or economically to monitor at every location of interest or predict future levels using this approach alone. In order to achieve estimates of air quality on both wider spatial and temporal scales, the use of air quality dispersion modelling is becoming more important.

It was intended to carry out a study to model levels of air pollutants over the Leicester area using air dispersion models, and compare the estimated levels with measurements from existing automatic and non-automatic monitoring data. The model was used as the tool to examine various aspects of the process of review and assessment of air quality, required under Part 4 of the Environment Act 1991. The study of air dispersion

models was achieved by two approaches: completing the emission database and numerical analysis between modelled data and monitored data.

Validation of air dispersion models in urban context was generally lacking. The aim of this project was to validate the applicability of the air dispersion models to predicting air quality indicators in the urban context. The objectives of the project were as follows:

- An emission database was set up and guidelines for the creation and application of emissions inventories for air dispersion modelling were developed;
- Modelled values against measured values of pollutant concentrations, using case studies in Leicester, were compared;
- Various modelling facilities in the model against measured data were tested. The study focused on pollutants associated with traffic flows;
- The performance of air dispersion model ADMS_Urban i.e. its strengths and weaknesses and its absolute accuracy, were analysed;
- The methodology of air quality model validation and application in an urban setting was developed;
- The future air quality scenarios were predicted and accessed.

CHAPTER 2 LITERATURE REVIEW

2.1 NEEDS FOR MODEL DEVELOPMENT AND APPLICATION

As noted in Chapter 1, air quality models have been applied in support of environmental decision making. As a further objective, trends of ongoing work towards better and more reliable models will be discussed in this chapter.

In the past, model development evolved in parallel to the clarification of the potential for the practical use of models. It is to a large extent iterative between the overall process of users adapting to the availability of new models and model developers becoming aware of specific needs for new model types for practical applications (DETR, 1997g).

The rapid growth of the public awareness concerning the need for environmental protection and for sustainable development led in recent years to increased political pressure towards more accurate impact assessment studies (DoE, 1994). With regard to the atmospheric environment, this implies a demand for better and more reliable models.

2.2 REVIEW OF AIR DISPERSION MODELS

2.2.1 Types of Air Dispersion Models

De Leeuw et al. (1995) demonstrated that models describing the dispersion and transport of air pollutants in the atmosphere could be distinguished through various features. For example, on the spatial scale (global; regional-to-continental; local-to-

regional; local), on the temporal scale (episodic models, (statistical) long-term models), on the treatment of the transport equations (Eulerian, Lagrangian models) and on the treatment of different processes (chemistry, wet and dry deposition).

Air dispersion models can be classified into the following categories. (More detailed mathematical descriptions and schematic representations of air dispersion models can be found in Appendix A.)

Gaussian models

The Gaussian plume model is the most common air pollution model (Zannetti, 1993). It is based on the assumption that the plume concentration, at each downwind distance, has independent Gaussian distributions both in the horizontal and in the vertical axes. Gaussian models have been modified to incorporate special dispersion cases. A simplified version of the Gaussian model, the Gaussian climatological model (Zannetti, 1993), can be used to calculate long-term averages (e.g. annual values).

Eulerian models

The transport of inert air pollutants may be simulated by the aid of models which numerically solve the atmospheric diffusion equation (Dobbins, 1979), i.e. the equation for conservation of mass of the pollutant (Eulerian approach). Such models are usually embedded in meteorological models. Eulerian models include refined sub-models for the description of turbulence (e.g. second-order closure models and large-eddy simulation models).

Lagrangian models

The Lagrangian approach consists in describing fluid elements that follow the instantaneous flow. They include all models in which plumes are broken up into elements such as segments, puffs or particles. Lagrangian models use a certain number of fictitious particles to simulate the dynamics of a selected physical parameter (Stull, 1988). Particle motion can be produced by both deterministic velocities and semi-random pseudo-velocities generated using Monte Carlo techniques (procedure employed to obtain numerical solutions to mathematical problems by means of random sampling). Hence, transport caused by both the average wind and the turbulent terms due to wind fluctuations is taken into account in Lagrangian models.

Chemical module

Several air pollution models include modules for the calculation of chemical transformation. The complexity of these modules ranges from those including a simple, first-order reaction (e.g., transformation of sulphur dioxide into sulphates) to those describing complex photochemical reactions. Several reaction schemes have been proposed for simulating the dynamics of interacting chemical species (Seinfeld, 1986). These schemes have been implemented into both Lagrangian and Eulerian photochemical models. In Eulerian photochemical models, a three-dimensional grid is superimposed to cover the entire computational domain and all chemical reactions are simulated in each cell at each time step. In the Langrangian photochemical models a single cell (or a column of cells or a

wall of cells) is advected according to the main wind in a way that allows the injection of the emission encountered along the cell trajectory.

Stochastic models

Stochastic models are based on statistical or semi-empirical techniques to analyse trends, periodicities, interrelationships of air quality and atmospheric measurements, and to forecast the evolution of pollution episodes (Bacci, 1981). Several techniques are used to achieve this goal, e.g., frequency distribution analysis, time series analysis, Box-Jenkins and other models, spectral analysis, etc. Stochastic models are intrinsically limited because they do not establish cause-effect relationships (Zannetti and Switzer, 1979). However, statistical models are very useful in situations such as real-time short-term forecasting where the information available from measured trends in concentration is generally more relevant for immediate forecasting purposes than that obtained from deterministic analyses.

2.2.2 Introduction to Model Packages

There are many air quality dispersion models commercially available. Specific models deal with point, area or line air pollution sources and a number of studies of their use have been made (Dabberdt et. al. 1995, and Benson, 1986, 1992). Most of them, as a set of computer software, often have a graphic interface for users to carry out modelling function i.e. input and output. In this section, short descriptions are given for the commonly used air dispersion model software.

OSPM *(Hertel, et al., 1989a)*

In the Operational Street Pollution Model (OSPM) model, concentrations of exhaust gases are calculated using a combination of a plume model for the direct contribution and a box model for the re-circulating part of the pollutants in the street. OSPM has been developed at the National Environmental Research Institute (NERI), Denmark. The model includes a simplified description of flow and dispersion conditions in streets. In spite of the simplifications, the model is able to simulate the dependence of air pollution levels on meteorological conditions, such as wind speed and wind direction. OSPM also includes a chemical sub-model which is used to calculate the conversion of NO to NO_2 using actual meteorological observations and estimations of emissions. The model provides hourly values of concentrations at prescribed receptor points in the street.

R91 *(DETR, 1997g)*

This Gaussian model was developed by a working group led by the UK National Radiological Protection Board (NRPB) in 1979. It has been used in past by UK regulatory bodies (especially the nuclear industry) as a reference model. R91 originally consisted of nomograms, but a PC version called DISTAR is commercially available; other PC versions include STACKS (encoded by the Meteorological Office) and PLUMES (used by the Environment Agency). DISTAR can only treat flat terrain and cannot model building wake effects, although reports by NRPB show how the basic R91 model can include these effects. The model calculates hourly, monthly and annual averages, but there is no percentile post-processor. It uses statistical meteorological data. DISTAR can treat both dry and wet deposition.

Industrial Source Complex (ISC) *(EPA, 1992)*

This is a USA Environmental Protection Agency multi-source Gaussian model, capable of predicting both long-term (annual mean) and short-term concentrations arising from point, area and volume sources. Effects of buildings can be considered using its BREEZE facility. The model has urban and rural dispersion coefficients, and percentile concentrations can be calculated using the percent post-processor if sequential meteorological data are used. ISC can handle up to 1000 sources and 10,000 receptors. It is widely used in the USA for the validation of industrial sources and has been updated over the years to remain compatible with PC systems.

Atmospheric Dispersion Modelling System (ADMS) *(CERC, 1996)*

ADMS is mainly a Gaussian plume model which can handle multiple sources. The concentration profiles of this multi-source dispersion model are assumed to be Gaussian in neutral and stable conditions but non-Gaussian profiles are adopted in convective conditions to allow for the skewness of the vertical velocity distribution. Specific features include the ability to treat both dry and wet deposition, building wake effects, complex terrain, and coastal influences. ADMS allows the use of point, area, volume and line sources, and can predict both long-term and short-term (down to one second mean) concentrations. Urban and rural dispersion coefficients are included, and percentile calculations are possible.

The version called ADMS_Urban can handle up to 1500 line (i.e. traffic) sources, and includes a street canyon option. It is marketed as a tool for urban air quality management. ADMS_Urban is the model used in this study.

AirViro *(DETR, 1997g)*

The AirViro system includes both a Gaussian plume and Eulerian grid model. Unlike most Gaussian models which rely upon meteorological information collected from a single site, the AirViro model describes a pattern of small-scale winds based upon the surface characteristics. The system differs from the other PC-based models in that it requires a UNIX workstation and requires complex geographic and meteorological configuration by the software supplier. The AirViro model interfaces with a sophisticated emissions database capable of accepting point sources (i.e. stacks), area sources and line sources (i.e. traffic) and detailed diurnal/seasonal/production variations of emissions (both traffic and industrial). This system can be applied using a number of Gaussian model options, and a street canyon model option.

UAM *(Ames et al., 1985; Chico and Lester, 1992)*

The Urban Airshed Model (UAM) is an urban scale, three dimensional, grid type numerical simulation model. It is an Eulerian model which calculates the concentrations of both inert and chemically reactive pollutants. At each integration time step, typically in the order of five minutes, the terms in the equation representing the different atmospheric processes (e.g. chemistry or diffusion) are solved separately in several steps using the numerical integration technique for the given process.

This is a widely used photochemical air quality model recommended by the US EPA for performing analysis and setting policy for Ozone abatement. UAM originates form the early 1970's when photochemical smog over large urban areas became major environmental issues. The UAM is coded in standard Fortran and the early versions were

run on mainframe computers. More recently the predominant platform has been UNIX workstations.

2.2.3 Limitations of Air Quality Models

Dabberdt et al (1995) indicated that although atmospheric models are vital in air quality assessment studies, their limitations should always be taken into account. Only when reliaable information on emissions is available, can models be used for estimating past, present and future air quality. The contribution of source regions, economic sectors etc. to the ambient levels can be deduced from model calculations by their selective use in the emission database. Uncertainties in model results may be large; uncertainties are introduced by both the model concept and by the input parameters (emission data, meteorology). The model results may be representative to a limited degree. In most models an implicit spatial and temporal average is introduced which may not allow a direct comparison with measurements at one location at a given moment.

2.3 APPLICATION AREAS OF AIR QUALITY MODELS

Four groups of model application areas are defined and their requirements are briefly discussed in this section.

2.3.1 Regulatory Purposes

In nearly all European countries models are currently in use for regulatory purposes (Olesen, 1995c). Model results are used in issuing emission permits (usually for single sources) or for environmental impact studies related to, for example, industrial plants and

new highways. In general terms, models in this application area have to provide spatial distribution of high episodic concentrations and of long-term averaged concentrations for comparison with air quality guidelines (Longhetto, et al., 1981). A wide range of pollutants are modelled (e.g. SO_2, NO_2, suspended particles, and also toxic substances like heavy metals and organics).

In the framework of a European initiative on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes, Olesen and Mikkelsen (1992) provided standardised methods such as tools for model validation. Their tool kit included the reference data set, software and protocols for model validation.

2.3.2 Policy Support

For policy support, the effect of abatement measures need to be forecasted by the models; this may require that the models also provide reliable results under pollution conditions which differ strongly from the present situation developed (Wadsworth et al., 1995).

2.3.3 Public Information

The role of models in providing information for the public is expected to grow. Requirements for models for public information parallel to a large extent those for policy support as far as concerns assessment studies. For on-line information to the public on air quality and the possible occurrence of smog episodes, air quality forecasting models are

needed. However, no standardised forecast models have been achieved so far (De Leeuw et al., 1995).

2.3.4 Fundamental scientific research

One of the major objectives for scientific research is the description of dynamic effects and the simulation of complex chemical processes involving air pollutants (De Leeuw et al., 1995). Until recently, the type of model for scientific research proved in most cases to be unsuitable for practical applications, as their requirement on computational effort was too high for application in the air quality management level for local authorities. De Leeuw et al. (1995) also indicated that, due to the tremendous hardware development, however, the situation is rapidly changing in favour of complex research type models. Therefore, models of this type are not only valuable for identifying limitations and gaps in simpler policy oriented models, they could also be used as proper policy supporting models in the near future.

2.4 REVIEW OF THE VALIDATION OF AIR DISPERSION MODEL

2.4.1 Importance of Model Validation

Despite the increasing interest in urban air quality problems, only limited has been conducted research to date on the validation of air dispersion models in an urban context. A great deal of study, including computer simulation, monitoring, and field testing, is required to analyse and quantify the air pollution distribution across the urban arena.

Analysing the potential for the practical use of mathematical models for air quality assessments implies investigating (1) what kind of statements can be made with the aid of models and (2) what is the accuracy of these statements.

The former approach is considered easier because it does not require more than understanding of the characteristics and the range of application of a model. In addition to that, a quantification of the accuracy of the model results presupposes insight into

- input data accuracy and how this affects the accuracy of model results
- uncertainties in model assumptions and parameterisations
- methodologies for judging to what extent model results represent reality.

As a consequence of the above, model validation should be considered an indispensable part of the model development process. An already validated model should be subject to a genuine evaluation procedure in order to ensure that potential users can assess the degree of reliability and accuracy inherent in the given model. In order to test the ability of a model, its results must be compared with experimental data. Hence validation work is an essential part of the development of any model.

The way to evaluate air pollution models seems to be straightforward: model predictions are compared against appropriate measurements. In spite of the simplicity of this method, Irwin et al. (1988) discussed that there are considerable difficulties both in properly defining the validation procedure and in interpreting its results. The validation datasets and methods should be ideally tailored to the specific application. Furthermore, deviations between model results and observations may be caused by various reasons, such as shortcomings in model assumptions and parameterisations, errors and inaccuracies in

input data (in particular emission data and meteorological data), uncertainties related to the stochastic nature of atmospheric processes (Venkatram, 1983).

Valuable experience of model validation has already been collected for simple models. A series of workshops were organised by the Steering Committee on "Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes" (Olesen, 1995b). One of the objectives is to test validation procedures for single source short-range atmospheric dispersion models (Olesen and Mikkelsen, 1992). Several steps have been taken during the past few years with regard to models assuming homogeneous terrain and inert pollutants. Specifically, a "Model Validation Kit" was created as the basis for the work on model validation. Being a collection of three experimental data sets (sites at Indianapolis, Kincaid and Copenhagan) and suitable software, this "Model Validation Kit" was meant to serve as a common frame of reference. This kit has been used for a common validation exercise involving five models (e.g. Kretzschmar et al., 1994). Some useful information emerged from this exercise, including the points below:

- the identification of strengths and weaknesses of models,
- the clarification of problems with model validation procedures and
- the need for continued model validation.

2.4.2 Components of Model Validation

Irwin (1982) indicated that model validation could include two parts: scientific review and validation with field data. It is necessary to state specific model validation objectives before the validation. Examples of objectives would include some aims, such as:

what types of sources are best characterised by the model; are chemical reactions being characterised.

One component of a model validation is to have a review of the modelling science to verify whether the construct of the model is reasonable and defensible for the stated validation objectives. For example, the characterisation of atmospheric processes is complex, but the set of modelling assumptions have to be limited to a reasonable amount.

Comparison of modelled concentration with observed field data provides a means for assessing model bias and precision. Due to the large anticipated stochastic variations of the atmosphere and the limited supply of validation data sets, there are some practical limits in assessing model performance. Therefore, the conclusions reached in the scientific review have particular relevance in deciding whether a model can be applied for conditions anticipated in the model validation objectives.

Two other methods that are supportive of model validation efforts are:

Verification of software

From Olesen and Mikkelsen (1992), a useful method that is to have a review in which the mathematics described in the technical description of the models are compared with the numerical coding, to ensure that the software faithfully implements the mathematics. Often the solution to a set of modelling algorithms will include or require numerical software (Olesen, 1997).

Sensitivity analysis

Irwin et al (1987) stated that performing sensitivity analyses can gain the response of a model to input variation. An example of this technique is to systematically vary one or more of the input parameters to determine the effect on the modelling result. Results from sensitivity analyses provide useful guidance. Some input parameters account for the greatest sensitivity in the modelling output. The sensitivity analyses also provide a view of what to expect for model output in conditions where validation data is not available.

2.4.3. Steps in Statistical Validations

As Irwin and Rosu (1988) indicated, two steps are important in the validation process. One is to understand the model to be validated, while the other is to choose data sets for model validation.

Understanding the Model

Irwin (1988) explained that some fundamental understanding of the underlying principles and concepts is important to the validation process. Therefore, before validating a model, the user should develop some understanding of the basis for the model and its operation.

Air quality simulation models can generally be distinguished by their scientific basis, by the range of pollutants and types of sources they can model, and by the extent of temporal or spatial detail they can accommodate in inputs, calculations and outputs. Some examples of understanding the different models are discussed as below.

From the study of Dabberdt et al (1995), air quality simulation models may be specified for a particular pollutant or in general terms. This distinction is important, because for example, particle-phase pollutants may behave differently from gas-phase pollutants. Particulate matter is subject to coagulation, chemical reaction at surfaces, gravitational settling, deposition, re-suspension and interception, implication, and deposition removal by vegetation, whereas some gaseous pollutants are subject to sorption and, in some cases, de-sorption processes.

Binkowski (1995) discussed the difference between short-term simulation and long-term simulation models. Short-term air quality simulation models predict atmospheric concentrations for averaging times that range from a few minutes to about an hour. Whereas long-term (sometimes called seasonal) models predict time-averaged atmospheric concentrations for a season or longer. If a long-term simulation model is to be validated, a statistical description of the frequency of occurrence of various atmospheric conditions and an average characterisation of emissions of each source is needed.

It is also found that it is not the case that increasing complexity in the treatment of the pollutant transport will provide more accurate predictions (Calder, 1976). Therefore a basic understanding of the underlying principles, the nature and extent of the inputs required, the inherent limitations, and the types of outputs provided are very important.

Choosing Data Sets for Model Validation

A fundamental requirement for a model validation exercise is that the data used for the validation process should be independent of the data used to develop the model. In

general, the following series of steps from Olesen (1995c) can be used in choosing data sets for model validation (suitable for validation of "single plume" situation):

- select validation field data sets appropriate for the applications for which the model is to be validated,
- determine the required levels of temporal detail (for example, minute-by-minute or hour-by-hour) and spatial detail (for example, vertical or horizontal variation in the meteorological conditions) for the models to be validated, as well as existence and variations of other sources of the same pollutant within the modelling domain,
- find or collect appropriate data for estimation of the model inputs and comparison with model outputs.

In principle, the information required for the validation process includes not only measured atmospheric concentrations but also measurements of all model inputs (Olesen, 1998). Model inputs typically include: emission release characteristics (physical stack height, stack exit diameter, pollutant exit temperature and velocity, emission rate), mass and size distribution of particulate emissions, upwind and downwind effect characteristics (for example, land-cover, surface roughness length), daytime and night time mixing heights, and surface-layer stability. However, in practice, suitable data for all the required model inputs are rarely available. Sometimes, it is required to collect additional data is required to enable proper estimation of inputs. A number of assumptions may be made when modelling even the simplest of situations. These assumptions, and their potential influence on the modelling results, should be identified in the validation process.

2.4.4. Difficulties in Model Validation

There are some essential problems which make model validation difficult. Venkatram (1988) and Olesen (1997) summarised the major difficulties in model validation as the following.

The appropriate validation method depends on the context of the application. An array of methods, useful for various purposes, should be available. However, in practice, the appropriate validation method cannot be uniquely defined.

Users want models to apply to a broad range of conditions, whereas the data sets used for design and verification of models have many limitations, e.g. input data sets are limited and can only reflect few of the possible scenarios. Also, there are not many comprehensive and high quality data.

The atmospheric dispersion processes are stochastic but models can be expected only to predict ensemble averages, not the results of specific realisations. These difficulties have also been discussed in papers by Olesen (1995a; 1995b, 1992) and Hanna (1993). A number of measures intended to overcome these difficulties have been pointed out. A general conclusion from these findings suggested it would greatly enhance the productivity of the modelling validation, if tools for model validation were made generally available, so that the practising modelling community would be able to use a common frame of reference.

2.5 REVIEW OF METHODOLOGIES FOR ASSESSING MODEL PERFORMANCE

2.5.1 Introduction of Validation of Dispersion Models

The performance of dispersion models can be estimated by comparing their predictions against field measurements. Irwin and Smith (1984) used tracer experiments are to evaluate the capability of plume models to properly simulate transport and diffusion. Comparison between model outputs and measurements were performed using both qualitative data analysis techniques and quantitative statistical methods (Irwin and Smith, 1984). Normally, the output of dispersion models is plotted against measurements and simple parameters such as the correlation coefficient are computed. High correlation values (a rare result) indicate that the model is good, low correlation (the most common case) that the model is poor. However, it is now clear that the problem is not so simple.

First of all, there are measurement errors. More importantly, even error-free measurements possess space and time limitations that prevent their use beyond their representative regions around the monitoring point. These representative regions are often very small and the comparison of measurements with averaged model output is inappropriate (Zinsmeister and Redman, 1980). Second, certain statistical parameters, such as the correlation coefficient, can provide misleading results (Zannetti and Switzer, 1979). Third, and most important, models rely upon emission and meteorological inputs. Often the errors in the determination of these inputs fully justify the disagreements between the predictions and observations (Irwin et al. 1982).

In the last decade, several methods for systematic statistical validation of air quality model performance have been proposed by Venkatram (1982, 1983). They provided some specific guidelines on the use of statistical tools in air quality applications. A summary of their recommendation was provided in Fox's papers (Fox, 1981, 1984). Fox (1984) also explained, for practical applications, several statistical parameters that can be used to evaluate pairs of predicted and observed concentrations, Among them are:

- The bias, i.e. the average difference of predicted minus observed values.
- The gross error, i.e. the average of the absolute difference.
- The variance of the difference.
- The correlation coefficient between predicted and observed values.
- The regression line, which ideally should have slope one and intercept zero.
- Frequency distribution analysis of the difference.

Finally, another point to be considered is the use of graphic methods for performance validation. In many cases, qualitative examinations of large datasets may reveal associations and patterns etc., which are hidden by summary statistics.

2.5.2 Raw Time series and Correlation Coefficient

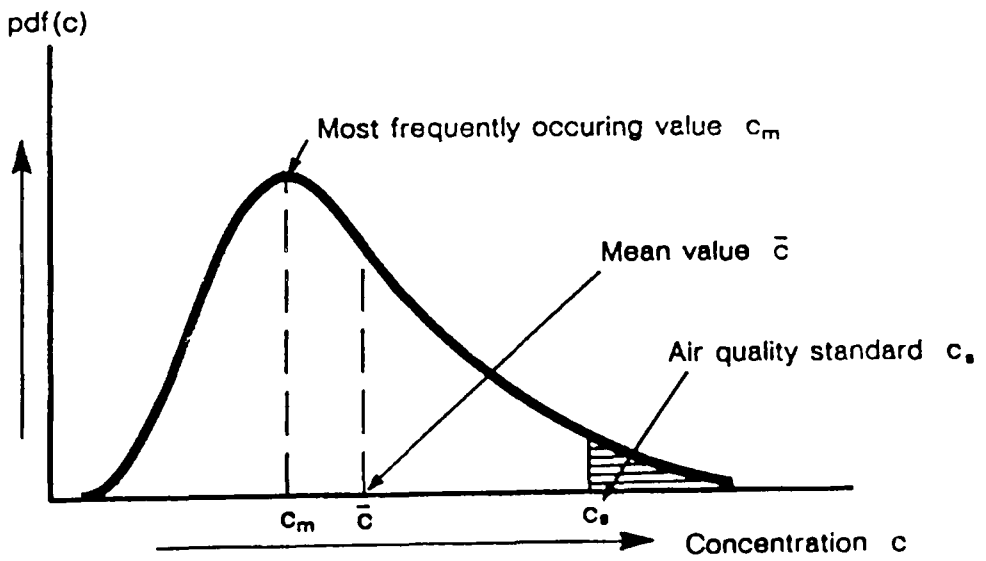
Time series analysis aims at the analysis of data arranged in a time sequence, either in the time domain (e.g. Box-Jenkins methods, Box-Jenkins, 1976) or in the frequency domain (e.g. spectral analysis). Irwin and Rosu (1988) provided some popular methods: such as, Box-Jenkins spectral analysis, regression method, trends analysis and principle component analysis.

These approaches used in a "black box" mode, for example, time series of concentrations are analysed without any other information, simply to evaluate their intrinsic variations and without attempting any physical explanation (Lee et al., 1994). Or, they can be used in a "grey box" mode, in which other parameters, for example meteorological and emission terms, are included.

2.5.3 Frequency Distributions

Puttock (1978) demonstrated that there is a fundamental similarity among the histogram of urban air pollutant concentrations sampled distributions when utilised to fit air quality data. As noted by Seinfeld (1986), " air pollution concentrations are inherently random variables because of their dependence on the fluctuations of meteorological and emission variables." The probability density function pdf(c) gives the probability pdf(c) dc and the concentration c, of a certain species at a particular location during a certain period, as between c and c+dc (see Figure 2.1).

Figure 2.1 Example of application of the pdf to calculate the probability of exceedence of air quality standard Cs. (source: Seinfeld, 1986)



The validation of the pdf has received more attention in air pollution statistical studies because its determination is useful in regulatory applications based on the concept of air quality "standards," i.e., ambient concentration values that should not be exceeded.

Several frequency distribution functions have been proposed and used to fit air quality measures. Georgopoulos and Seinfeld (1982) discussed and summarised several of them, including: Log-normal, Gamma, Three-parameter log-normal, Three-parameter beta, Four-parameter beta and Pearson etc. The most common distribution is the log-normal distribution. The log-distribution has been studied by several authors, including Larsen (1971), whose work identified the following relations, sometimes referred to as Larsen's laws: pollutant concentrations are log-normally distributed for all averaging times; median concentrations (50^{th} percentile) are proportional to averaging time raised to an exponent; maximum concentrations are approximately inversely proportional to the averaging time raised to an exponent.

Frequency distributions (e.g. probability density function) are mostly used to assess the probability of occurrence of high concentration values (e.g. exceedences). Therefore, it is important that these distributions are accurate at their "right tail" than elsewhere. It is well known, however, that extreme values are the most affected by uncertainties (Hanna, 1993).

2.5.4 Statistical Indices

Two widely used air quality model validation indices are Normalised BIAS (NBIAS) and Normalised Mean Square Error (NMSE). Weighted Normalised Mean Square Error of the Normalised Ratios (WNNR) and Normalised mean square error of distribution

of Normalised Ratios (NNR) are two new tools proposed by Poli and Cirllo (1993). A brief discussion of these indices is as follows.

Normalised BIAS (NBIAS)

The NBIAS is defined as (Fox, 1981)

$$NBIAS = (\overline{C}_m - \overline{C}_o)/\overline{C}_o \qquad (2\text{-}1)$$

$\overline{C}_m$ and $\overline{C}_o$ are the modelled and the observed concentrations respectively, over-bar indicating the averaging procedure with respect to the sampling points. Defining the ratios as:

$$K_i = \overline{C}_{mi}/\overline{C}_{oi} \qquad (2\text{-}2)$$

and

$$S_i = \overline{C}_{oi}/\overline{C}_o \qquad (2\text{-}3)$$

Where i refers to the i-th receptor, also define $\hat{K}_i$=1/K_i (if K_i>1) and $\hat{K}_i$=K_i (if K_i<=1)

As it is evident, a perfect model would give NBIAS =0, while NBIAS >0 (or <0) the model on average overestimates (or underestimates) the observed concentrations. The NBIAS can be written as:

$$NBIAS = \sum_i S_i(K_i - 1)/\sum_i S_i \qquad (2\text{-}4)$$

The value of the NBIAS index does not only depend on the ratio K_i, but also on the ratio S_i, i.e. on the specific set of the observed concentrations. Therefore, it is not right to compare the values of NBIAS index found with respect to different sets of observed concentrations.

The value of the NBIAS index can disappear or almost disappear even in the case of evident disagreement between modelled and measured concentrations. Hence this index should be used only to evaluate the "on average " behaviour of the model with respect to the overestimation or the underestimation of measured values.

The normalised mean square error (NMSE)

The normalised mean square error NMSE (Hanna, 1985) is defined as,

$$NMSE = (\overline{C}_m - \overline{C}_o)^2 / \overline{C}_m \overline{C}_o \qquad (2\text{-}5)$$

Where $\overline{C}_m$ and $\overline{C}_o$ are the single concentration values. NMSE can also be written as:

$$NMSE = \sum_i S_i^{\,2} (1 - K_i)^2 / \sum_i S_i K_i \qquad (2\text{-}6)$$

A perfect model would give NMSE=0, otherwise, the value of this index is always positive.

As in the case of the NBIAS index, the value assumed by the NMSE index does not only depend on the ratio K_i, but also on the ratio S_i, i.e. on the specific set of the observed concentrations. Therefore, it is not strictly correct to also compare the values of NMSE index found with respect to different sets of observed concentrations too.

Weighted Normalised Mean Square Error of the Normalised Ratios (WNNR)

The WNNR (Weighted Normalised Mean Square Error of the Normalised Ratios) is defined as (Poli and Cirillo 1993);

$$WNNR = \sum_i S_i^{\,2} (1 - K_i)^2 / \sum_i S_i K_i \qquad (2\text{-}7)$$

A perfect model would give WNNR =0, the value of this index always being positive.

As in the case of the NBIAS and NMSE indices, the value assumed by the WNNR index depends on the specific set of the observed concentrations: in fact the formula defining the WNNR index also contains the ratio S_i. Therefore, again, it is not strictly correct to compare the values of WNNR index obtained with respect to different sets of observed concentrations.

Normalised mean square error of distribution of Normalised Ratios (NNR)

The NNR is defined as (Poli and Cirillo 1993):

$$NNR = \sum_i (1 - K_i)^2 / \sum_i K_i \qquad (2\text{-}8)$$

A perfect model would give NNR=0, the value of this index always being positive.

The value assumed by the NNR index does not depend on the specific sets of observed concentrations, since in the formula defining this index the ratio S_i does not appear. Thus, contrary to the NBIAS, NMSE and WNNR indices, it is correct to compare the values of the NNR index obtained with respect to different sets of observed concentrations (Poli and Cirillo 1993).

The absence of the ratio S_i in the formula defining the NNR index also implies that this index gives the same 'weight' to all of the ratio K_i, relative to both low and peak observed concentrations. In other words, the NNR index gives the same relevance to errors on the whole scale of the observed concentrations.

Fractional Bias (FB)

For a plume model, the dispersing plume sometimes "expands" to an angle of the order of 10 to 20 degrees during transport downwind. With such a narrow plume, even a 4

degree error in estimating the transport direction can cause very large differences between predicted and observed concentrations paired in time and space (Irwin and Smith, 1984).

Hence, meaningful comparisons can not be accomplished by comparing observed and estimated concentration values paired in both time and space. By stratifying the data into dispersive regimes, meaningful comparisons can be made by comparing selected features of the predicted and observed concentration distributions. The Fractional Bias (FB) was selected for this reason. The normalised fractional bias FB (Irwin and Smith, 1984) is defined as:

$$FB = 2(\overline{C}_m - \overline{C}_o)/(\overline{C}_m + \overline{C}_o) \qquad (2\text{-}9)$$

where $\overline{C}_m$ and $\overline{C}_o$ are the modelled and observed average concentration values (normalised by dividing by the emission rate) for the quartile of values, respectively. FB varies between -2 and 2 with an optimum value of zero.

Cox and Tikvart (1990) explained the definition of $\overline{C}_m$ and $\overline{C}_o$ in forming the FB should be guided by the anticipated use of the models. For instance, if the model is to be applied to predict infrequently occurring maximum concentration values C_{max}, then C_{max} could be defined using the concept of a Robust Highest Concentration (Cox and Tikvart, 1990), which involves extrapolation from an exponential fit to the upper 5 to 10% of the concentration values. The experience of Irwin and Lee (1996) suggested that some additional improvement could be made by using $\log\overline{C}_m$ and $\log\overline{C}_o$, which relate more directly to $\overline{C}_m/\overline{C}_o$. The authors recommended consideration of using a Gaussian fit to each receptor arc in defining the maximum concentration measure.

2.5.5 Summary

The statistical methodologies for validating model performance reviewed in this chapter have generally been applied to single plume models for where specific plume trace data may be obtained. However, model validation in the urban context is relatively less well developed. In this study, application and validation of the air dispersion model ADMS_Urban in an urban setting, all of the statistical indices described above were considered inappropriate. For the purpose of air quality management, the cumulative performance of the model in terms of predicting exceedences is more important than the prediction of instantaneous values. A review of previous validation exercises of ADMS can be found in Chapter 3 (section 3.5).

CHAPTER 3 THE ADMS_URBAN AIR DISPERSION MODEL DESCRIPTION

3.1 INTRODUCTION To ADMS_URBAN

This study focuses on the application and validation of the air dispersion model ADMS_Urban, which has been developed by Cambridge Environmental Research Consultants Ltd. (CERC).

The Atmospheric Dispersion Modelling System (ADMS) is an atmospheric dispersion model for calculating short range dispersion from point sources. The system includes modules for plume rise, dispersion of particulates, and for the effect of buildings, hills, roughness variations and coastlines, as well as modules for predicting deposition, fluctuations in concentration, radioactive decay and doses from gamma radiation (CERC, 1996).

There are three versions of ADMS. The simplest is called ADMS-Screen which looks at worst-case scenarios. It can quickly tell the user if a proposed emissions source might be a problem. If this is the case a more detailed study can be undertaken using one of the other ADMS models. The most powerful model is ADMS_Urban. It can cope with thousands of emissions sources. (CERC, 1996).

ADMS 2.0 and ADMS_Urban can work with two other programs for handling data. The first of these is Surfer, which is a third-party product allowing a user to create a variety of useful 2-D and 3-D images and concentration profiles of dispersed pollution. CERC has

also provided a program which lets ADMS work seamlessly with the ArcView GIS package. (ADMS 3 is released in 1999).

The Urban version of the Atmospheric Dispersion Modelling System (ADMS_Urban) is a PC based model of dispersion in the atmosphere of pollutants released from the range of source types present in urban areas, namely industrial, domestic, and road traffic. The model treats these using point, line, and area and volume source (McHugh, et al., 1997).

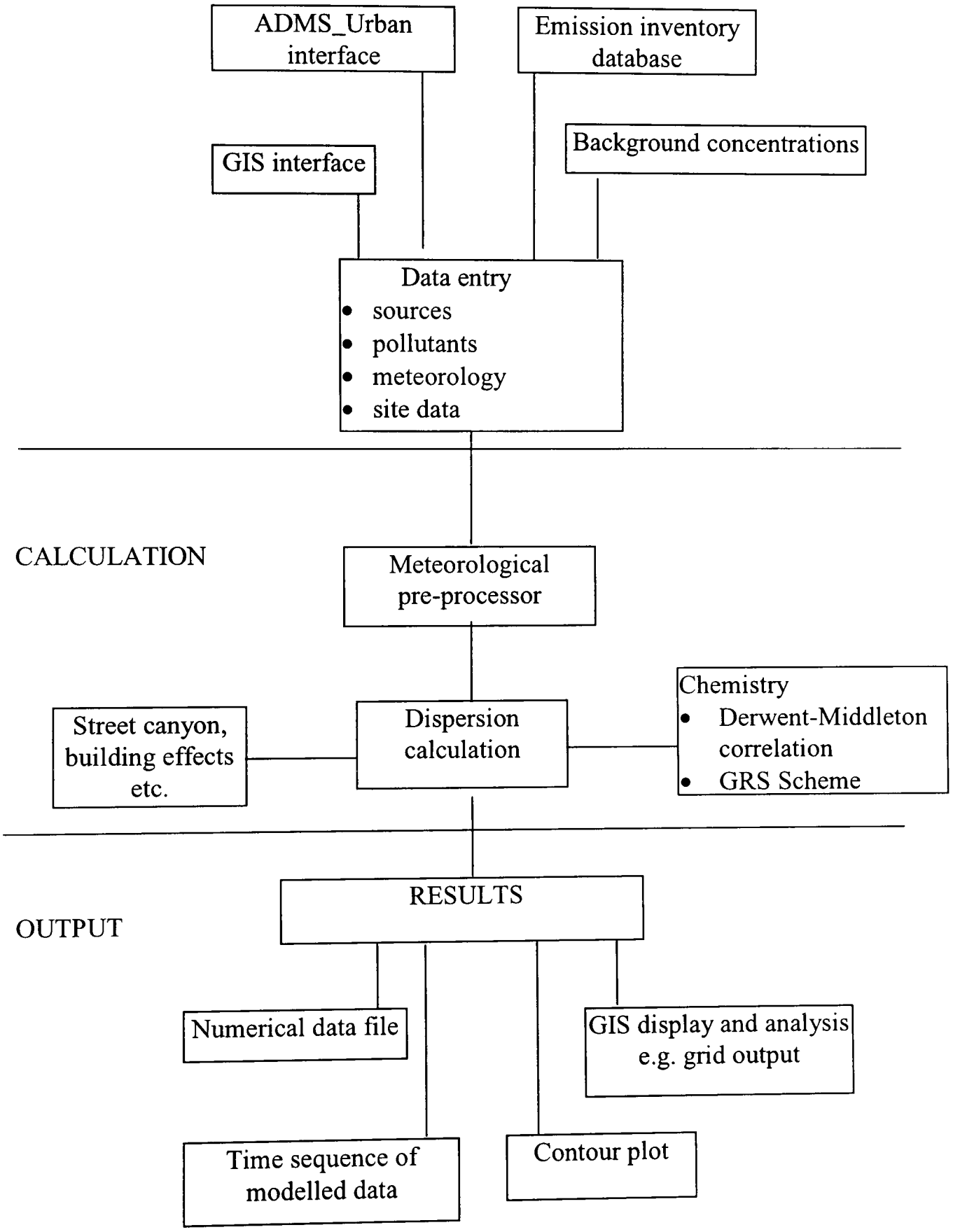
3.2 FUNCTIONALITY OF ADMS_URBAN

3.2.1 Outline of ADMS_Urban

ADMS_Urban combines the base model (ADMS model), which includes a line and area source model, with an integrated street canyon model, a chemistry model for predicting the conversion of NO to NO_2 and the generation of ozone and a traffic emissions database. Up to 1500 sources are permitted in the standard model, which calculates concentrations for up to 10 pollutants (McHugh, et al. 1997). The concentrations are calculated for averaging times appropriate for comparison with the EU, WHO (World Health Organisation) and EPAQS (Expert Panel of Air Quality Standard -UK) limits and guidelines values.

Figure 3.1 outlines the structure of the model, showing the options for entering data and for viewing the results. The options are intended to simplify the entry of what will typically be a large volume of data.

Figure 3.1 ADMS_Urban Model Structure



3.2.2. Input Module

The ADMS_urban model adopts an approach to boundary layer scaling based on the Monin-Obukhov length (which is a parameter that characterises the 'stability' of the surface layer) and boundary layer depth rather than on Pasquill-Gifford stability classes. This is a major difference between ADMS_Urban and other models used for air dispersion modelling in urban areas. The concentration profiles are assumed to be Gaussian in neutral and stable conditions but non-Gaussian profiles are adopted in convective conditions to allow for the skewness of the vertical velocity distribution, which allow for a realistic representation of the changing characteristic dispersion with height (Carruthers et al, 1992).

Meteorology input module

This section describes the range of meteorological data that can be entered into the model and the meteorology parameters that are calculated from the raw data by the meteorology pre-processor for use in the dispersion model. Meteorological data can be input to the ADMS_Urban model in two ways: (1) via a prepared meteorology file supplied by the user and (2) by entering one or more sets (lines) of data manually in the model file (CERC, 1996).

In (1), the meteorology input module reads the data from the meteorology input dataset and uses the pre-processing algorithms to calculate values of the various meteorological quantities required for running the dispersion model.

In (2), the minimum data required may be entered and the model will calculate the boundary layer height, a parameter required by this dispersion model. Alternatively, the

parameter boundary layer height, surface temperature and standard deviation of the wind direction may be entered in addition to the minimum. However, it is advised that these extra parameters should only be used if accurate values are known (CERC, 1996).

The meteorological input data sets can contain a variety of input meteorology parameters in ADMS_Urban. The minimum data requirements are wind speed (this would normally be a near surface wind (e.g. 10m), and wind direction plus one of the following:

- Reciprocal of Monin-Obukhov length
- Surface sensible heat flux $F_{\theta 0}$
- Cloud cover, time of day and time of year

If more than one of the latter three are supplied, the reciprocal of Monin-Obukhov length is used in preference to the others, i.e. the cloud cover, time of the day and time of the year are ignored. If cloud cover, time of day and time of year are the only data specified, then it is advised to add temperature and boundary layer depth to the variables in the meteorological file if accurate values are known (CERC, 1999). In addition, specifying temperature may also help to improve the module's estimate of the boundary layer height.

Additional meteorology input data that may be required by the model are (CERC, 1999):

- Precipitation rate, if wet deposition is to be calculated (unless a constant value of washout coefficient is specified).
- Frequencies with which particular conditions occur are needed for statistical meteorological data.

The complete list of possible input is shown in Table 3.1. The first column contains the symbols used to represent each parameter in the meteorology data file. The second

contains the representation of each parameter in standard notation. The asterisked parameters are those which may be entered as a line of input in the model file.

In Table 3.1, SI units used except where stated. α is a parameter representing the surface moisture available for evaporation. Typical values range from 1.0 for moist grassland to 0.0 for dry bare earth and 0.45 for dry grassland. 1.0 is the default value in the model (CERC, 1999).

Table 3.1 Variables to the Meteorology Input Model (source: CERC, 1999)

U	U	* Wind speed
UGSTAR	U_g	*Geostrophic wind speed normalised by the friction velocity
PHI	ϕ	* Wind direction (angle wind is coming from in degrees clockwise from north, e.g. 180' is a southerly wind
DELTAPFI	$\Delta\phi$	Geotrophic wind direction minus surface wind direction (degrees)
FTHETA0	$F_{\theta 0}$	Surface heat flux
RECIPLMO	$1/L_{mo}$	Reciprocal of the Monin-Obukhov length $L_{mo} = \frac{-U_*^3}{\kappa g F_{\theta 0}/(\delta C_p T_0)}$ Where k is von Karman's constant (=0.4), δ density and C_p specific heat capacity.
H	h	*Boundary layer depth
NU	N_u	Buoyancy frequency above the boundary layer
DELTATHETA	$\Delta\theta$	Temperature jump across the boundary layer top
T0C	T^c_0	*Near surface temperature (^{0}C)
P	P	Precipitation rate (mm/hour)
CL	C_l	* Amount of cloud cover (oktas)
R	r	Surface albedo
ALPHA	α	Modified Priestly-Taylor parameter (as defined in Holtslag and van ulden, 1983)
TDAY	t_{day}	*Julian day number
THOUR	t_{hour}	*Local time (hours)
FR	f_r	Frequency of occasions when these conditions occur (arbitrary units, e.g. percentage of occasions or number of hours per year).
SIGMATHETA	σ_θ	*standard deviation of mean wind direction (degrees)

In ADMS_Urban, the boundary structure is characterised by the two parameters, the boundary layer-height h and the Monin-Obukhov length L_{mo}. Value of these parameters corresponding approximately to the Pasquill-Gifford categories are shown in Table 3.2. "A" represents the most unstable condition and "G" represents most stable condition in P-G category.

Table 3.2 Values of h and L_{mo} corresponding approximately to the Pasquill-Gifford categories (source: CERC, 1999)

$U(ms^{-1})$	$L_{mo}(m)$	$1/L_{mo}$ (m^{-1})	H(m)	H/L_{mo}	P-G Category
1	-2	-0.5	1300	-650	A
2	-10	-0.1	900	-90	B
5	-100	-0.01	850	-8.5	C
5	∞	0	800	0	D
3	100	0.01	400	4	E
2	20	0.05	100	5	F
1	5	0.2	100	20	G

There is no exact correspondence between the Boundary layer parameters (h, L_{mo}) and the Pasquill-Gifford categories since many different values of h and L_{mo} may correspond to one Pasquill-Gifford category. The following category is used in the model (CERC, 1995):

Stability: Stable $h/L_{mo} > 1$

Neutral $(-0.3<h/L_{mo}<1)$

Convective $h/L_{mo}< -0.3$

As well as the data in the meteorological input data sets, the meteorological input module also requires certain other input data. These are roughness lengths and the height of the wind measurement. The typical values of surface roughness lengths are as a function of

land use, such as, surface roughness length is 1.0 for cities and woodlands, 0.5 for parkland or open suburbia, 0.3 for agriculture areas, 0.001 for sandy desert.

Multiple source module

A single source may have up to 10 pollutants and a pollutant, if particulate, may have up to 10 different particle sizes. The limit on the total number of particle sizes and gaseous pollutants defined is 250, that is

$$\sum_{i=1}^{NSRC} \sum_{j=1}^{NPOLL} \sum_{k=1}^{NPG} I_{ijk} \leq 250 \qquad (3\text{-}1)$$

where NSRC is the number of sources, NPOLL is the number of pollutants in a source, NPG is the number of particle sizes or gaseous species (always =1 for gaseous pollutant) for a pollutant, and I_{ijk} is an integer, value=1 if a source/pollutant/particle size or gas combination exists, value =0 otherwise (CERC, 1995).

Up to 1500 pollution sources are allowed in ADMS_Urban version 1.51. The source may be assigned to up to 5 groups and the integration of groups, sources and pollutants is explained below.

Group Module

Up to 5 groups are permitted. Each group may contain all sources, so that a source may be a member of more than one group, but a source can only appear once in any group. This is useful for predicting the pollution concentration of selected areas, e.g. postcode areas.

Sources

A source may be a point, area, volume or line source. The source is defined by its position, dimensions e.g. diameter, length or side length, height and emission characteristics, for example:

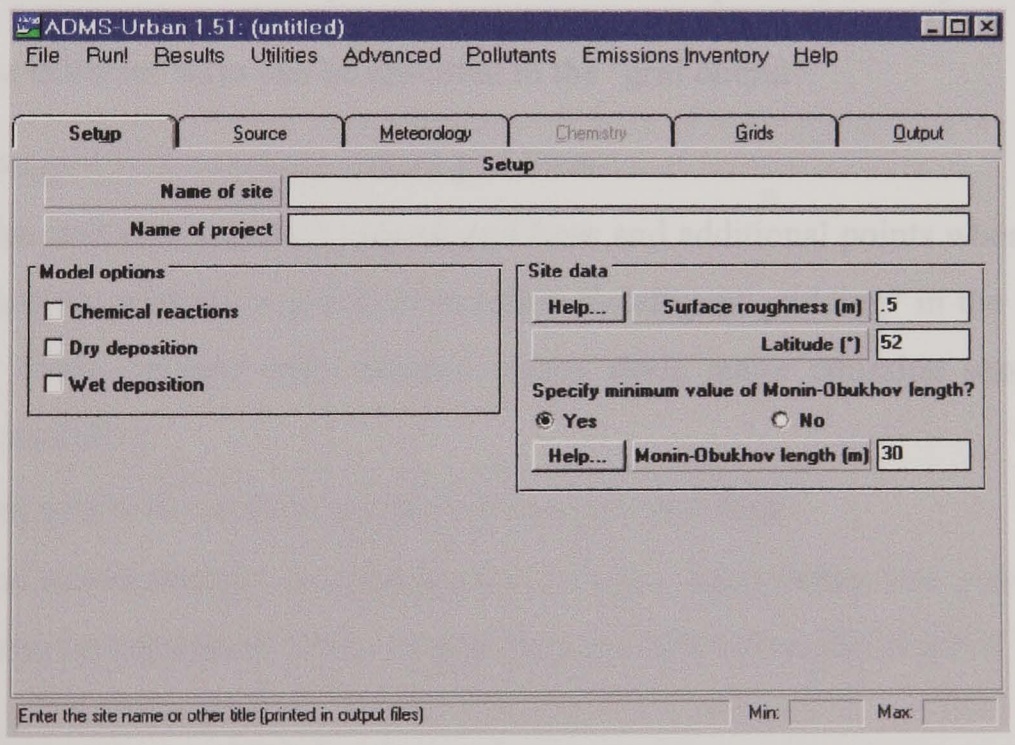
- Vertical velocity or volume flow rate.
- Temperature and molecular weight or density.
- Specific heat capacity.
- Each source may have up to 10 pollutants.

Pollutants

A pollutant is defined by a mass emission rate. If the pollutant is particulate, up to 10 different sizes may be defined, but if gaseous, only one species may be defined.

ADMS_Urban model interface is shown below.

Figure 3.2 ADMS_Urban 1.51 Interface (Screen Shot from ADMS_Urban)



3.2.3 Outputs

ADMS_Urban model has various output options. The output includes

- Calculations to compare with existing EU, WHO, and EPAQS (UK) limits and guideline: 15 min, hourly, 8- hourly, daily and annual average concentrations.
- Output to a GIS package to allow geographical analysis of the results.
- Viewing of model predictions and ambient air quality measurements.

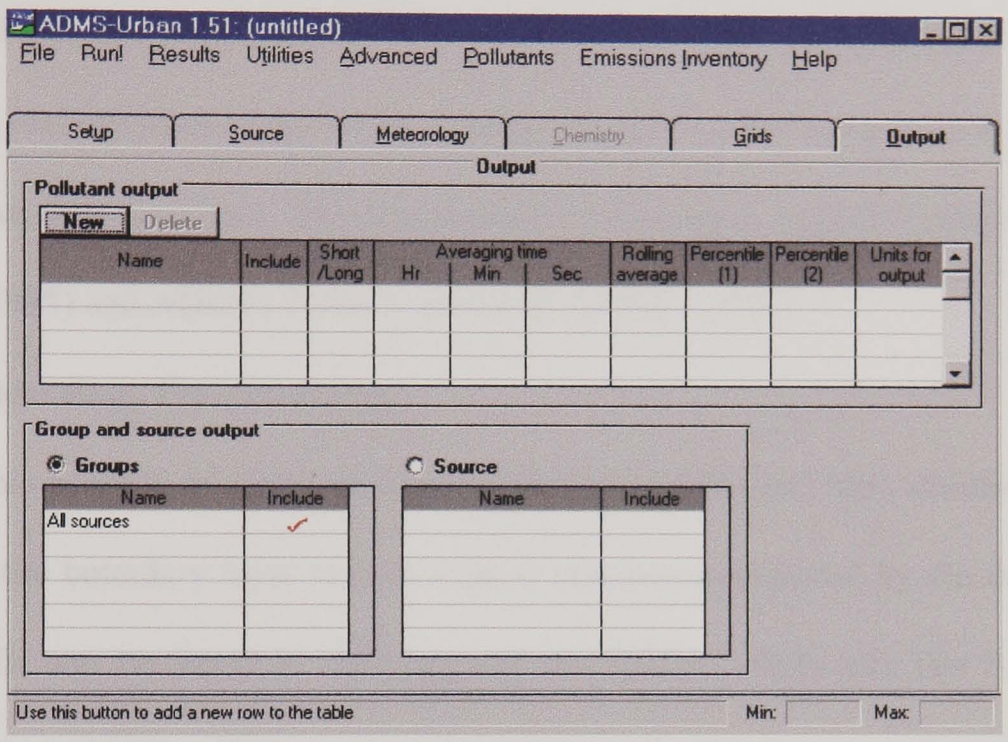
Used alone or in combination, these options allow the user to assess the impact of changes on ambient air quality, i.e. proposed traffic schemes, existing or proposed industrial sources and changes in domestic emissions, and to determine whether guidelines and limit values are being breached, or are likely to be breached (CERC, 1999). One of the options is called "grid output". It displays the calculated pollution values over a contour map by using a GIS (i.e. ArcView) software. The "grid output" allows the problem areas to be identified and is a tool in the presentation of results, especially to the public.

Four different ways can be specified in the "grid output":

- Cartesian grid with regularly spaced grid lines.
- Cartesian grid with regularly spaced grid lines and additional points where the pollutant concentration gradient is greatest (so called "intelligent gridding" in the ADMS_Urban model, which can add extra receptor points along major emission sources, i.e. main roads, junctions).
- Cartesian grid with variable spacing between the grid lines.
- Specified points defined in Cartesian co-ordinates. Grid output and output at specified points may be combined. Up to 32 grid lines are allowed in the X and Y directions at Z level.

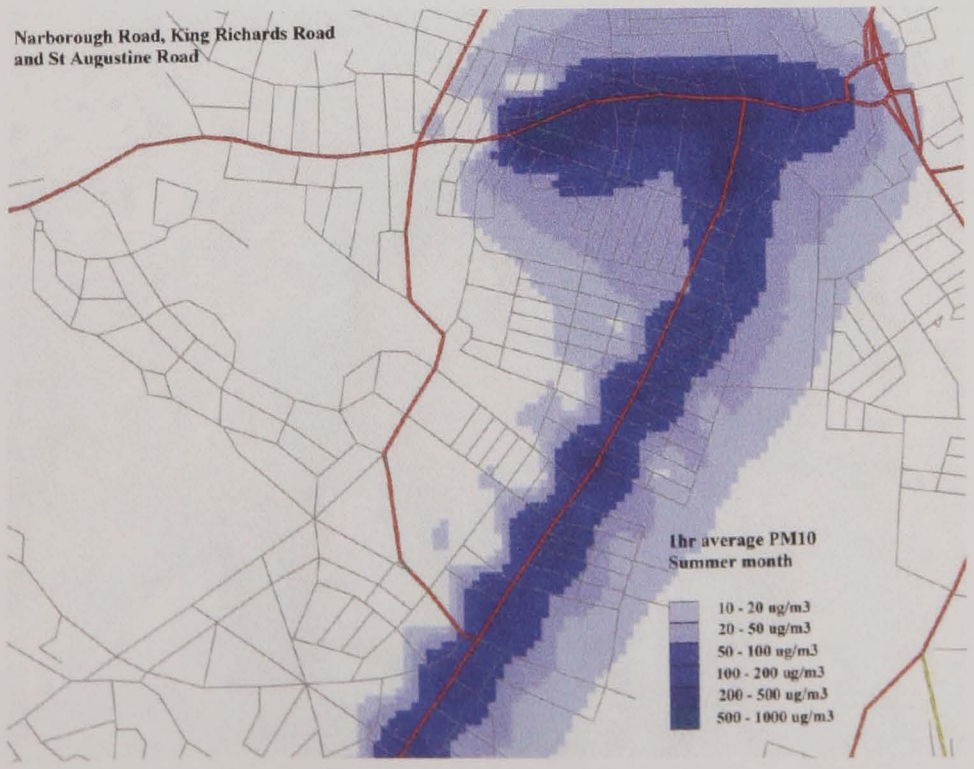
The output interface is shown in Figure 3.3.

Figure 3.3 ADMS_Urban1.51 Output Interface (Screen Shot from ADMS_Urban)



An example of ADMS_Urban grid output is shown in Figure 3.4. The output grid was defined along the major road, and the pollution levels along and around this road (illustrated by colour legend) are clearly presented.

Figure 3.4 Example of Prediction for Pollution Dispersion in Leicester using ADMS_Urban and ArcView



3.3 BASIC THEORY OF ADMS_URBAN

Some of the main modules are introduced here. They include the meteorology pre-processing, the parameterisation of the boundary layer, the methods of calculating mean concentrations, the plume rise module, dry deposition and wet deposition module etc. The advanced features such as the building effects module, street canyon module and chemistry module are also discussed. The description is based upon ADMS Technical Specification (CERC, 1995) and ADMS_Urban User Guide (CERC, 1999).

3.3.1 Meteorology Pre-processing

This module is called once for each hour's data and uses standard algorithms to calculate the boundary layer meteorological parameters required by the dispersion model. Full details can be found in Holtslag and van Uldan (1983) and The ADMS Technical Specification (1995). If the meteorology site is distant from the area of dispersion, the meteorology input module presents the option to modify the wind profile at the source by taking account of the surface roughness both at the meteorology site and the source. Output variables by the meteorological input module are shown in Table 3.3.

Table 3.3 Output by the Meteorology Input Module (source: CERC, 1999)

u_*	Friction velocity
U_g	Geostrophic wind speed
U_{g*}	Geostrophic wind speed normalised by the friction velocity
ϕ_0	Surface wind direction (angle wind is coming from in degrees clockwise from north, e.g. 180 is a southerly wind)
ϕ_g	Geostrophic wind direction (angle wind is coming from in degrees clockwise from north)
$\Delta\phi$	Geostrophic wind direction minus surface wind direction (degrees)
U	Wind speed - as obtained from the meteorology input dataset
ϕ	Wind direction - as obtained from the meteorology input dataset
w_*	Convective velocity scale if $F_{\theta_0} > 0$, $w_* = (gF_{\theta_0} h / \rho c_p T_0)^{1/3}$; if $F_{\theta_0} \leq 0$, w_* =0.
F_{θ_0}	Surface heat flux
$1/L_{mo}$	Reciprocal of the Monin-Obukhov length
H	Boundary layer depth
N_u	Buoyancy frequency above the boundary layer
$\Delta\theta$	Temperature jump across the boundary layer top
T_0	Near surface temperature (K)
P	Precipitation rate (mm/hour); P may be missing if insufficient input data are given.
F_r	Frequency of occasions when these conditions occur (arbitrary units, e.g. percentage of occasions or number of hours per year)
σ_θ	Standard deviation of mean wind direction (degree).

3.3.2 Parameterisation of the Boundary Layer

In ADMS, the boundary layer is characterised by the boundary layer height h and the Monin-Obukhov length L_{mo}. In unstable conditions, the Monin-Obukkov length is negative. Under such conditions, the magnitude of the length is a measure of the height above the

ground above for which convective turbulence, that is turbulent motions caused by convective motions, are more important than mechanical turbulence generally by friction at the earth's surface. In stable conditions the Monin-Obukhov length is positive. Then it is a measure of the height above the ground which vertical turbulent motion is greatly inhibited by the stable stratification. The Monin-Obukhov length is defined as (CERC, 1995)

$$L_{mo} = \frac{-U_*^3}{\kappa g F_{\theta 0} / (\delta C_p T_0)} \qquad (3\text{-}2)$$

where U_* is friction velocity at the earth's surface, $\kappa(= 0.4)$ is the von karman constant, g is the acceleration due to gravity, F_{θ_0} surface heat flux, δ and C_p are respectively the density and specific heat capacity of air and T_0 the surface temperature.

Vertical profiles of the following variables are expressed as functions of z/L_{mo} and z/h (CERC, 1995).

$u(z)$, du/dz, d^2u/dz^2	Mean wind, velocity and gradients
$\sigma_u(z)$, $\sigma_v(z)$, $\sigma_w(z)$	r.m.s. turbulent velocities
$\Lambda_v(z)$, $\Lambda_w(z)$	Turbulent length scales
$\varepsilon(z)$	Energy dissipation rate
$T_L(z)$	Langrangian time scale
$N(z)$	Buoyancy frequency
$T(z)$	Temperature
$\rho(z)$	Density

These variables are, in turn, called by the mean concentration, plume rise and building modules in ADMS_Urban.

3.3.3 Mean Concentrations

Averaging times

The mean concentration averaging time, or, sampling time t_s, specified in the model file is used to calculate the lateral spread due to changes in mean wind direction over the time t_s, unless is entered as a meteorological variable. t_s may take any value from 0 seconds to 24 hours. For a plume (continuous release) t_s = 1 hour is appropriate for many calculations. The concentration output is then the ensemble average hourly concentration.

Dispersion parameters

Research and field experiment have shown that the way the dispersion parameters vary with downwind distance from a point source depends in the states of the atmospheric boundary layer height (h), the height of the source (Zs) and the height of the plume as it grows downwind. Some reviews can be found in Hunt, Holroyd and Carruthers (1988). This approach is in contrast to older methods described in NRPB report R91 and used in ISC, in which the effect of the source height is not taken into account when calculating the width and depth of the plume (Hanna et al., 1989).

There is no general theory or even generally accepted semi-empirical expression that describes the dispersion from all source heights ($0<Zs/h<1$) in all conditions of atmospheric stability and over the complete range of distance from the source extending to about 30km downwind.

In ADMS_Urban, the approach adopted (Hunt et al, 1988) is first to use formulas that were developed for specific ranges of the parameters Zs/h, h/Lmo (stability) and x/h (downwind distance).

The distribution of the concentration profile is a Gaussian plume with reflections at the ground and the inversion layer (CERC, 1995), i.e.

$$C = \frac{Q_s}{2\pi\sigma_y\sigma_z U} e^{-y2/2\sigma_z y^2} \{e^{-(z-z_s)2/2\sigma_z^2} + e^{-(z+z_s)2/2\sigma_z^2} + e^{-(z+2h-z_s)^2/2\sigma_z^2} + e^{-(z-2h+z_s)^2/2\sigma_z^2} + e^{-(z-2h-z_s)^2/2\sigma_z^2}\} \quad (3\text{-}3)$$

Where C is the concentration; Q_s is the emission rate; σ_y and σ_z are the standard deviations (horizontal and vertical) of the plume concentration spatial distribution.

The stable and neutral boundary layer

All the turbulence in the stable boundary layer is assumed to be mechanically generated, i.e. there is no generation of turbulence due to convective motions. Usually the level of turbulence decreases with height, as the relative effects of stratification increase, although it can be enhanced by wave motions at the top of the boundary layer. However, the effect of the wave motions is not considered by ADMS_Urban.

The vertical dispersion parameter σ_z at the mean height of the plume, Z_m, is linked directly to the vertical component of turbulence, σ_w, and the travel time from the source, t, by the relationship (Hunt, et al.1988),

$$\sigma_z = \sigma_w t \{\frac{1}{b^2} + \frac{N^2 t^2}{1 + 2\gamma^2 Nt}\}^{-1/2} \quad (3\text{-}4)$$

where *N,* σ_w, and *U(z)* are the boundary frequency, the r.m.s. vertical velocity and the mean wind speed at height z respectively. Parameter γ represents the rate of mixing of the plume with the environment and the factor b ensures a smooth transition between the solution for surface releases and elevated releases.

The transverse dispersion parameters, σ_y, is given by:

$$\sigma_y^2 = \sigma_{yt}^2 + \sigma_{yw}^2 \qquad (3\text{-}5)$$

in stable flows, $h/L_{mo}>1$

$$\sigma_{yt} = \sigma_v\, t\, (1 + (15.6)^{1/3}\, u_*\, t\, L_{mo}/h^2)^{-1/2} \qquad (3\text{-}6)$$

and in neutral flows, $-0.3< h/L_{mo}<1.0$,

$$\sigma_{yt} = \sigma_v\, t\, (1 + (15.6)^{1/3}\, u_*\, t\, /h)^{-1/2} \qquad (3\text{-}7)$$

σ_{yw} is equal to $\sigma_{\theta x}$. σ_θ is either specified as a meteorology input parameter, or the meteorology pre-processor calculates an effective σ_θ using

$$\sigma_\theta = 0.65\sqrt{7T/U_{10}} \qquad (3\text{-}8)$$

where T is the averaging time in hours, (=1 hour). The spreading due to turbulence σ_{yt} is assumed to become linear with respect to time in stable flows when h/L_{mo} is large, as increasingly large scales diffuse the plume as it travels downwind.

The Convective boundary layer

Field experiments of diffusion from elevated sources in the convective boundary layer (Hanna, 1985) have confirmed earlier laboratory and computational studies (e.g. Lamb 1980) that the form of the vertical profiles of concentration are skewed and significantly non-Gaussian for there meteorological conditions.

Vertical distribution

In the convective boundary layers (CBL) the probability distribution of the vertical velocity and the concentration distribution is non-Gaussian, or skewed. The non-Guassian distribution ensures that, for elevated sources, the height at which the concentration is

maximum descends as the plume moves downwind, whiles its mean height ascends. After the height of the maximum concentration reaches the ground it can rise again.

Transverse Spread

The transverse dispersion parameter is calculated as two parts, the first for dispersion due to convection σ_{yc}, the second due to mechanically driven turbulence σ_{yn}, the algorithms used are:

$$\sigma_{y_c} = \sigma_{v_c} t \left(1 + \frac{t}{h} o.75^{1/3} w* \right)^{-1/2} \tag{3-8}$$

$$\sigma_{yn} = \sigma_{vn} t \left(1 + \frac{t}{h} 15.6^{1/3} w* \right)^{-1/2} \tag{3-9}$$

σ_{vc} and σ_{vm} are the r.m.s horizontal velocities due to convection and mechanically driven turbulence respectively. An additional term σ_{yw} may be included to allow for the variation in the wind direction.

The total spread is given by

$$\sigma_y{}^2 = \sigma_{y_n}{}^2 + \sigma_{y_c}{}^2 + \sigma_{y_w}{}^2 \tag{3-10}$$

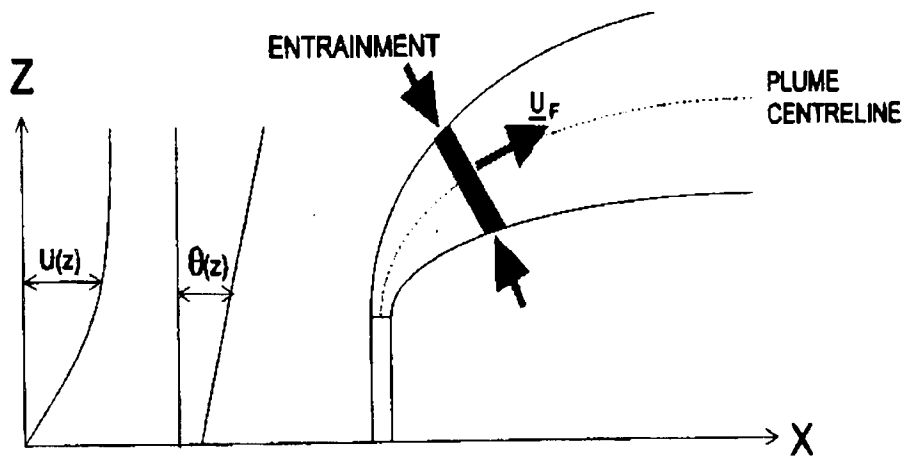
3.3.4 Plume Rise Module

The plume rise module predicts the rise trajectory and enhanced dilution of a continuous emission of hot gaseous material, e.g. from a stack. The underlying theory is a top-hat, integral model, and includes penetration of inversions.

Integral conservation equations are solved for the fluxes of mass, momentum and heat, assuming the plume to be a continuous, bent-over cone of circular cross-section over

which plume properties velocity, density, etc. are uniform. The external velocity and temperature fields may vary with height. The plume rise diagram is shown in Figure 3.5.

Figure 3.5 Plume Rise (source: CERC, 1999)



The plume rise module is initialised from source conditions: exit diameter and emission velocity and density. The equations are then solved numerically using a variable internal time-step. The plume may completely penetrate the inversion, so that no material remains in the boundary layer, in which case, the plume rise module is not called again although all other calculations continue.

3.3.5 Dry Deposition and Wet Deposition Module

The rate of deposition is assumed proportional to the near-surface concentration; that is:

$$F = V_d\, C\,(x, y, 0) \qquad (3\text{-}11)$$

where F is the rate of deposition per unit area per unit time, C is the predicted airborne concentration and V_d is the deposition velocity. It contains a diffusive part, known as the deposition velocity V_d' (equation 3-12), and an element due to the gravitational settling, V_s,

the terminal velocity of a particle. They are related to the overall deposition velocity, V_d by the equation,

$$V_d = \frac{V_s}{1 - \exp(-V_s / V_d')} \qquad (3\text{-}12)$$

One or both of V_d' and V_s, may be input directly or estimated by the diagram on the basis of gas type, or particle size and density.

3.3.6 Area, Volume and Line Sources

Area, volume and line sources with the following geometry are treated in ADMS_Urban.

Area sources

Co-ordinates of area sources must be quadrilaterals and are specified by the co-ordinates of each of their vertices. The mass emission entered in the "Emissions" section of the model file must be in mass units/m^2/s.

Volume sources

Volume sources are considered to be area sources with vertical extent, and therefore they may not have an efflux velocity or volume flow rate, i.e. no plume rise. The base area of a volume source is described in the same way as an area source. A vertical extent is also supplied, with the volume source extending above and below the centre of the source. The mass emission entered in the interface must be in a mass units/m^3/s.

Line sources

Line sources are specified by the positions of their two end points and a width, which may be zero, see Figure 3.6. They are assumed to lie in a horizontal plane. The width is only used if plume rise is "on" i.e. the line source has a non-zero efflux velocity or

volume flow rate, and in that case the result depend on the width L_1. Therefore care should be taken in defining problems with plume rise from line sources. The mass emission must be in mass units/m/s.

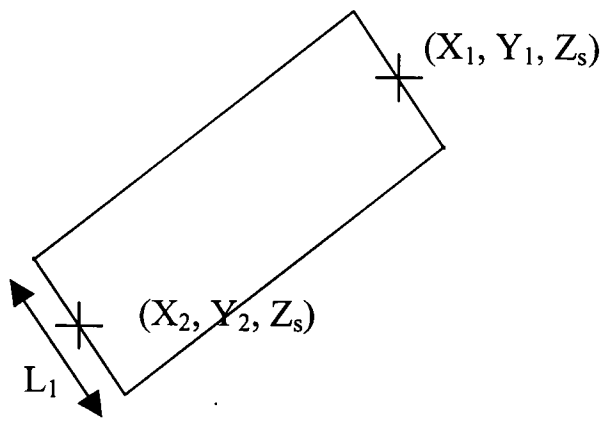


Figure 3.6 Parameterisation of line sources (source: CERC, 1999)

In the ADMS-Urban model, scheme for calculating concentrations from area sources is defined in terms of the concentration from a point source. And the integration of the point source formula to give the concentration due to a finite length, crosswind line source, the equation is used as i.e.

$$\overline{C}(x, y.z) = \frac{Q_s e^{-y^2} / 2\sigma_y{}^2 x}{\sqrt{2\pi}\sigma_y(x)} f(z, p(x)) \qquad (3\text{-}13)$$

(All terms are previously defined.)

The calculation method is described as follows:

- For each meteorological condition: calculate σ_y (10m), the lateral spread at the mean plume height 10m downstream of the source.
- Then for each output point: 1) remove redundant parts of the source that cannot possibly contribute to the calculated concentrations, using σ_y(10m); 2) divide the source

into elements which are approximately the same along wind distance from the source; 3) replace each of these elements with a cross wind line source of equivalent source strength and 4) calculate the concentration by summing over the source elements using crosswind formulae of point and line sources.

3.3.7 Statistics - Long Term Averages

Long term averages of hourly means and percentiles can be calculated using meteorological data which have been statistically analysed, e.g. by the Meteorological Office (and therefore have a frequency or weighting attached to each meteorological condition), or from raw data. The latter data may be sequential. The module outputs long term average mean concentrations, long term average mean deposition fluxes, long term average mean activity (radioactivity) and long term average percentile concentrations.

To calculate the concentration at each point corresponding to a specified percentile p at ground level, i.e. C(x, y, z), the values of C(x, y, z) at one point for each combination of meteorological variables are considered along with their frequency of occurrence f. First of all the concentration values are arranged in descending order (i.e. highest at the beginning, lowest at the end) and the values of f rearranged accordingly. Then, starting at the highest concentration, the frequencies are summed until their cumulative value is (100-p)/100.

3.4 ADVANCED FEATURES

The advance features of ADMS_Urban are summarised below.

3.4.1 Building Effects Module

The Building Effects Module is used to calculate the dispersion of pollution from sources near large structures, out to a distance of about 60 times the building height. The ADMS_Urban model of building effects has the following main features:

- A building is defined in ADMS_Urban by the user in terms of its height, length, width and orientation to the north. For each wind direction, representative streamwise and crosswind lengths are calculated by the program. A complex of buildings is reduced to a single rectangular block whose dimensions are a function of the height of the major building (identified by a tick in the user interface) and representative streamwise and crosswind lengths.
- The disturbed flow field consists of a re-circulating flow region or cavity in the lee of the building, with a diminishing turbulent wake downwind.
- Concentrations within the well-mixed re-circulating flow region are uniform and based upon the fraction of the release which is entrained.
- The concentration and deposition are set to zero within the user defined buildings.
- Concentrations further downwind are the sum of those from two plumes: a ground-level plume from the re-circulating flow region and an elevated plume from the non-entrained remainder. The turbulent wake reduces plume height and increases turbulent spread.

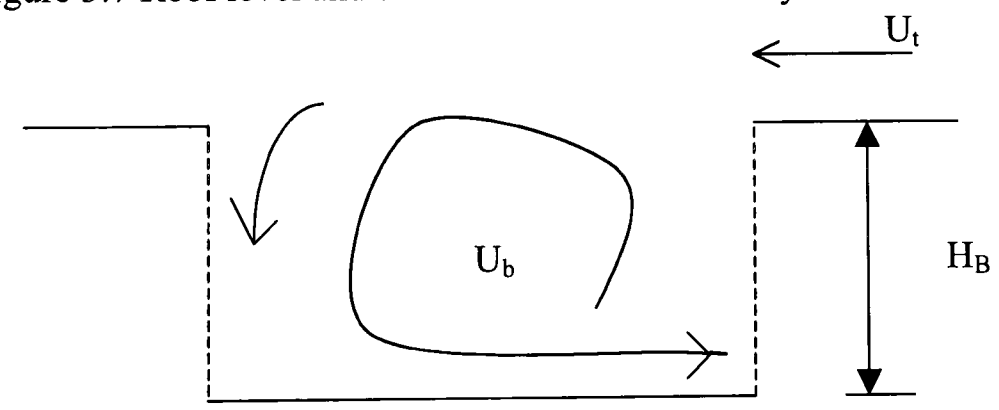
The Building Effects Module interacts with the rest of ADMS_Urban, using the underlying concentration profiles, but with modified plume parameters.

3.4.2 Street Canyon Module

The street canyon model which is incorporated into ADMS_Urban is based on the Danish model OSPM. OSPM (Operational Street Pollution Model) was developed at the Danish National Environmental Research Institute (NERI). It is described in a series of papers (Hertel, et. al, 1989a, 1990, 1989b, 1989c) and has been validated against Danish and Norwegian data. It uses a simplified flow and dispersion model, with a Gaussian plume model.

From Apsley (1988), the canyon model is used for calculating the concentration at points which lie in roads lined with buildings with heights greater than 2m. Concentrations inside the road tend to the non-canyon results in the limits as the canyon height is reduced to zero or the road width increased to over twice the canyon height. Concentrations at points outside the canyon are identical with those which would be obtained if the road were not a canyon. A schemetic illustration of roof level and street winds in a street canyon can be found in Figure 3.7, where Ut is the wind speed, H_B is canyon height, the wind is re-circulating in the canyon in wind speed U_b.

Figure 3.7 Roof level and street winds in a street canyon



3.4.3 Chemistry Module

There are two chemistry functions available in ADMS_Urban, one is the Derwent-Middleton Correlation, another is the Generic Reaction Set.

The Derwent-Middleton Correlation (DMC)

When this option is selected, output concentrations of NO_2 are calculated from input NOx emissions. The concentration of NO_2 calculated using the following function derived from Derwent and Middleton (1996), where concentrations are hourly average concentrations in ppb.

$$[NO_2]=2.166-[NOx\ (1.236-3.348A + 1.933A^2- 0.326A^3)] \qquad (3\text{-}14)$$

where $A = \log_{10}((NOx)$. The equation is valid in the range 9ppb to 1141.5ppb.

The equation is used to subdivide calculated concentrations of NO_x into NO_2 and NO. This is the simpler approach to derive NO_2 and NO from NO_x. It does not predict the pollution concentrations by taking the account of chemical reactions.

The Generic Reaction Set

As noted in Chapter 1, vehicles and industrial sources emit a complex mixture of chemicals including many organic compounds e.g. VOCs (Volatile Organic Compounds) and oxides of Nitrogen which are involved in reactions with Ozone.

It is beyond the scope of a fast practical model to account for all the chemical reactions. Therefore a scheme is used which models the important reactions involving Nitrogen, VOC's and Ozone (CERC, 1999). The ADMS_Urban model adopted the Generic Reaction Set (GRS) of equations (Venkatram et al., 1994), which is a semi-empirical

photochemical model which reduces the complicated series of chemical reactions involving NO, NO_2, Ozone and many hydrocarbons to just seven:

(i) $ROC + h\nu \rightarrow RP + ROC$

(ii) $RP + NO \rightarrow NO_2$

(iii) $NO_2 + h\nu \rightarrow NO + O_3$

(iv) $NO + O_3 \rightarrow NO_2$

(v) $RP + RP \rightarrow RP$

(vi) $RP + NO_2 \rightarrow SGN$

(vii) $RP + NO_2 \rightarrow SNGN$

where:

$h\nu$ = Sun Light

ROC = Reactive Organic Compounds

RP = Radical Pool

SGN = Stable Gaseous Nitrogen products

SNGN = Stable Non-Gaseous Nitrogen products

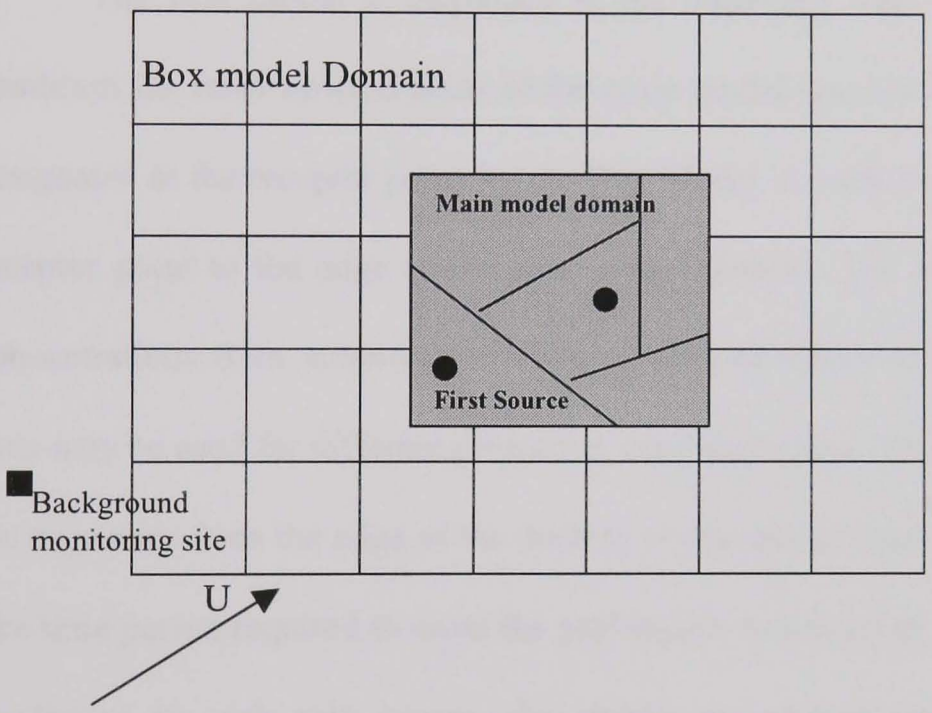
Equations (iii) and (iv) above represent exact chemical reactions, which happen very quickly. The other equations are approximations.

The chemistry scheme in ADMS_Urban consists of two modules. The first models chemical reactions that occur only in the main model domain. The main model domain contains all the individually defined sources, receptor points and output grids. For each set of input meteorological data, the time taken (Δt) for background pollutants to travel from the most upwind point of the main model domain to the first (most upwind) source is calculated. The chemistry scheme is then applied to the background pollutants over the period Δt to calculate background concentrations at the first source. All background concentrations downwind of the first source are assigned the values that occur at the first

source, so that chemical reactions are not applied twice to these pollutants. The scheme is only applied to points that are affected by source emissions within the main model domain.

The second module consists of a simple Lagrangian box model, which is used to calculate background concentrations for the air approaching the main model domain. This allows the main ADMS model to be nested within a larger domain such as a large urban conurbation, where the effects of NOx and VOC emissions over the whole area need to be considered (Figure 3.8).

Figure 3.8 Schematic showing the main model nested within large area box model domain (source: CERC, 1999).



A major restriction on the complexity of the box model is computational time, as it is used for a large number of sequential meteorological data sets. For this reason a single layer "Box" model with a regular grid is used in ADMS_Urban. Meteorological parameters and emissions are assumed to be constant over the grid square.

The governing equation for the box model is

$$\frac{dC(t)}{dt} = \frac{F_e}{H_{mix}} - \frac{V_d C(t)}{H_{mix}} \qquad (3\text{-}15)$$

where C(t) is the concentration of the chemical species at time t, H_{mix} is the depth of the atmospheric boundary layer, V_d is the applied deposition velocity and F_e is the emission flux of the species.

The solution of this equation for a time period Δt (assuming steady state conditions) is given by

$$C(t_0 + \Delta t) = C(t_0) * \exp\left\{-\frac{\Delta t * V_d}{H_{mix}}\right\} + \frac{F_e}{V_d} * \left[1 - \exp\left\{-\frac{\Delta t * V_d}{H_{mix}}\right\}\right] \qquad (3\text{-}16)$$

The Box model is employed in the following way. For each prevailing weather condition the most upwind point of the main model domain is calculated and this point is designated as the receptor point for the Box Model. A back trajectory is calculated from the receptor point to the edge of the Box Model domain. The box model is initialised using concentrations from automatic monitoring sites or values specified by the user. Different sites may be used for different prevailing wind directions. The Box Model is then run along the trajectory from the edge of the domain to the receptor point, grid square by grid square. The time period required to cross the grid square is estimated, and by assuming steady state conditions in each grid square, the change in concentration due to emission and dry deposition is computed easily using the above formulation. The algorithms used to determine values in the current grid square are the same used by the FRAME atmospheric transport model (Singles et al., 1997).

Once the new concentrations have been calculated for the current grid square, the GRS chemistry scheme is applied to calculate the change in concentrations due to chemical processes. The chemistry scheme uses an adaptive time stepping scheme which determines the time step dependent on the maximum rate of change of concentration occurring amongst all the pollutants. This allows the chemistry module to proceed quickly when concentration changes due to chemical reactions are low, and more slowly when detailed and rapid chemistry is occurring.

The "age" of a pollutant in the air column is then calculated, for a time period Δt (terms are defined as same as in equation 3-15)

$$Age = \frac{1}{C(t_0 + \Delta t)} * \left[\frac{\Delta t * F_e}{V_d} * \left[1 - \exp\left\{ - \frac{\Delta t * V_d}{H_{mix}} \right\} \right] + \frac{C(t_0) * H_{mix}}{V_d} * \left[1 - \exp\left\{ - \frac{\Delta t * V_d}{H_{mix}} \right\} \right] \right] \quad (3\text{-}17)$$

where the first part of the equation in parenthesis refers to material emitted from the current grid square (which is relatively new material), and the second term refers to material advected in from the previous grid square (which is relatively older material).

This scheme is used for each grid square on the trajectory. For the final grid square, which contains the receptor point, a smaller time step is estimated to be the time of travel from the edge of the grid square to the receptor point. Pollutant concentrations at the receptor point are then used as background values in the main ADMS model.

3.5 VALIDATION OF ADMS

ADMS and ADMS_Urban have been subject to a number of validation studies. They are summarised below.

3.5.1 The Comparison with Kincaid Dataset

Comparisons between the predictions of ADMS (version 1.04) and some observations were made during the three experiments (Carruthers et al 1993). The comparisons were made between ADMS (version 1.01) and a more detailed set of the Kincaid data (187m power plant stack in Illionis). Results show that ADMS tends to over-predict close to the source. A possible explanation for this could be that ADMS does not take account of the residual buoyancy which buoyant plumes have once they impact on the top of the boundary layer. Further comparisons with the Kincaid data showed better agreement between the observations and the model (Carruthers et al 1993). That study again highlights the difficulty of making useful comparisons where the quality of the data is uncertain and the intrinsic variability is large. Various statistical measures of model performance also obtained using the BOOT (Olesen, 1995b) package. It was suggested that the model performed satisfactorily, but given the various uncertainties, such statistical measures may not be sufficient to conclude whether a model performs well or not.

3.5.2 The Relative and Absolute Performance of ADMS and R91/ISC-ST

The results presented in Carruthers et al (1991), lead to the following conclusions:

- ADMS provides a more reliable prediction than R91/ISC-ST (see Chapter 2, section 2.2.2 about R91 and ISC) of the location and magnitude of the maximum ground-level concentration in convective conditions, for elevated sources.

- ADMS is based on a better-founded parameterisation of the state of the atmospheric boundary layer and more realistic descriptions of plume rise and dispersion than is R91/ISC-ST.
- Comparisons based solely on ground-level concentrations over a limited range of conditions may not be sufficient to demonstrate the relative performance of dispersion models.

3.5.3 Contrasting Methods for Validating ADMS Using the Indianapolis dataset

Carruthers et al. (1998a) presented results of validation of ADMS against the Indianapolis data set (84m power plant stack situated on the edge of Indianapolis) using the BOOT (Olesen, 1995b) statistical package. They found that the model results showed good agreement with the daytime measurements and these results were insensitive to a change in roughness length from 1m to 3 m and minimum Monin-Obukhov length from 1m to 200m. They reported that this insensitivity was anticipated, as the meteorological conditions prevailing during the day were convective. At distances close to the source concentrations were sometimes over-predicted and at distances greater that about 3km concentrations were under-predicted. The night-time results consistently underestimated even when meteorological conditions were assumed to be neutral, suggesting there were significant anthropogenic heat sources which were not being modelled but were responsible for the high rate of dispersion at height.

3.5.4 Validation of ADMS_Urban

ADMS_Urban is based on the dispersion model ADMS which was extensively validated (Carruthers et al, 1993, 1996, 1998a). However, the validation of air dispersion

models in the urban context has not been investigated to the same degree. ADMS_Urban has been used for approximately half of the pilot studies of air pollution carried out recently in the UK (Carruthers et al., 1998b). The study of three areas, London, Neath/Port Talbot, Swansea, and Belfast were briefly reported. From emission data available there was good agreement between predicted and measured values of main pollutants, SO_2 and NO_x. For Benzene and PM_{10}, the predicted values significantly underestimated concentrations. In Neath/Port Talbot and Swansea this might have been due to the neglect of sources of particulate and an underestimate of emitted benzene levels. In Belfast study no clear reason for under estimate in PM_{10} levels was found (Carruthers, et al., 1998b).

3.5.5 Discussion of ADMS_Urban

ADMS_Urban is a skewed Gaussian model which characterises the boundary layer in terms of the Monin-Obukhov length rather than the previous Pasquill-Gifford stability scheme (Carruthers et al., 1992). As such, it is considered to be more accurate than the Pasquill-Gifford type models as errors in the Pasquill's dispersion figures have been acknowledged to be possibly in the order of $\pm$25% (Beychok, 1998). Significant errors remain in ADMS_Urban, however, including those introduced by the plume rise equations which can again be in error by $\pm$20%. There are also errors in the calculations of averaging time which become particularly important for the assessment of transient effects such as odour nuisance. Many assumptions are made about the dispersal of the plume which may not hold in areas of complex topography. The Gaussian model also relies upon a wind speed to calculate dispersion. For periods of calm, a "dummy" wind speed is introduced in ADMS_Urban. In summary, the small errors in the parameters of a Gaussian model can

lead to very large variations in the model's predictions. A study by Beychok (1998) indicated that "It is probably realistic to expect consistent predictions of real world concentrations within a factor that may be as high as ten".

CHAPTER 4 DATA FOR VALIDATION AND MODEL INPUT

4.1 INTRODUCTION

A wide variety of monitoring techniques have been used to monitor air pollution levels in Leicester over the years. The smog problems of the 1950's resulted in more intensive monitoring of smoke and sulphur dioxide levels in the 1960's and 1970's (LCC, 1991). However, the most significant development in recent years was the introduction of an advanced automatic monitoring station in 1994, providing data of high quality and high resolution for the first time. This is now part of the national Automatic Urban Network (AUN). The data from the Leicester AUN was used for the validation of ADMS_Urban model.

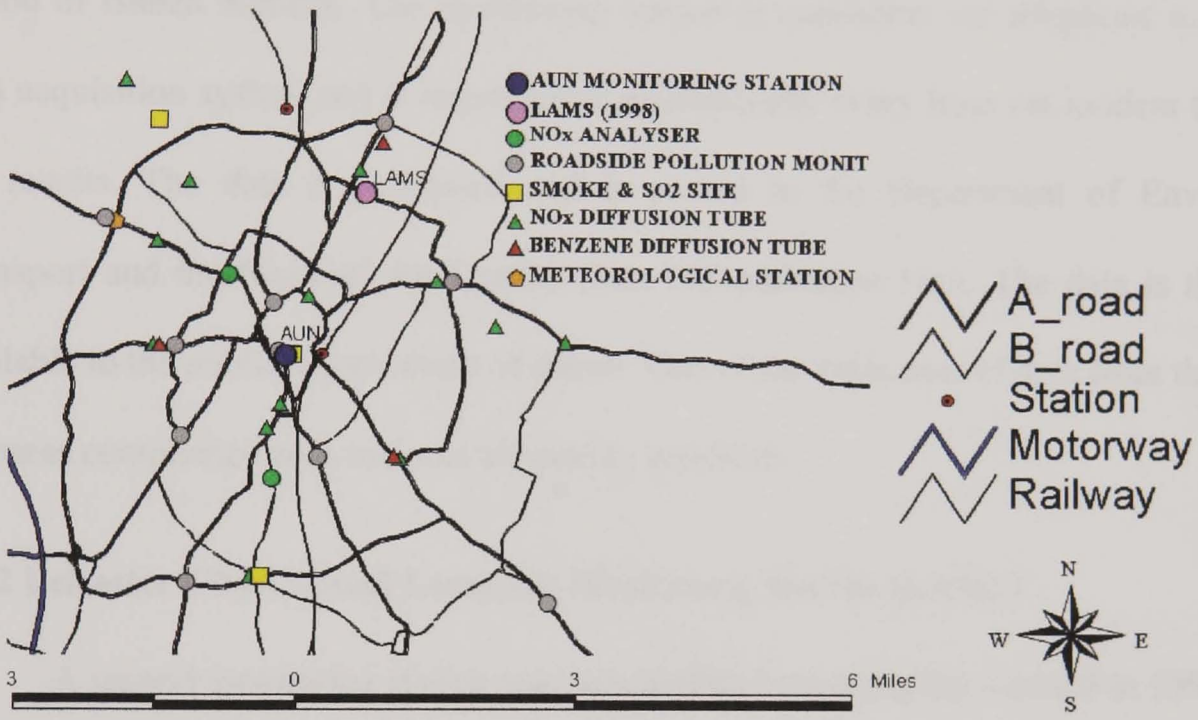
Whilst there are a number of well established techniques for measuring the concentrations of pollutants in the atmosphere, it is not always possible to identify their sources or the relative importance of multiple sources. The use of an emissions inventory may be the only way of doing this (Hutchinson and Clewley, 1996). An emissions inventory forms the most important input for air quality models. Knowledge of the significant sources of air pollutants is essential before any action can be taken to improve air quality in a particular area.

This chapter investigates the availability of data for validation and the construction of an emission inventory for the city of Leicester.

4.2 AIR QUALITY AND METEOROLOGICAL MEASUREMENTS FOR LEICESTER

All of the monitoring facilities currently used in Leicester are described in this section. The distributions of air quality monitoring stations in Leicester can be found in Figure 4.1.

Figure 4. 1 Air Quality Monitoring in Leicester



4.2.1 Automatic Urban Network (AUN)

The Automatic Urban Network (AUN) is a national network of UK Government and local authority monitoring stations. The AUN uses real-time continuous analysers to monitor ambient levels of five principal pollutants:

- Sulphur dioxide (SO_2)
- Oxides of nitrogen (NO, NO_2 and NO_x)
- Ozone (O_3)

- Carbon monoxide (CO)
- Particulate (PM_{10})

The Leicester City Centre monitoring station is located in the piazza of New Walk Centre, Welford Place and has been operational since 1994. This site is classed as an urban background location, which represents the levels of pollutants to which large numbers of people are exposed.

Pollution levels are continuously measured and levels are calculated for averaging period of fifteen minutes. The monitoring station is connected via telephone to a central data acquisition system and is interrogated automatically every hour via modem to retrieve the results. The data is processed and is passed to the Department of Environment, Transport and the Regions' Air Quality Data Dissemination Unit. The data is then made available to the public via a variety of means. One of the main uses of data from the AUN is to assess compliance with national air quality standards.

4.2.2 Leicester City Council Local Air Monitoring Station (LAMS)

A second monitoring station was acquired by Leicester City Council in 1995. This is virtually identical in specification to the AUN monitoring station, but is re-locatable. It is known as the Local Air Monitoring Station (LAMS). It uses real-time continuous analysers to monitor ambient levels of five principal pollutants:

- Sulphur dioxide (SO_2)
- Oxides of nitrogen (NO, NO_2 & NO_x)
- Ozone (O_3)
- Carbon monoxide (CO)
- Particulate (PM_{10})

However, unlike the AUN monitoring station which has continuously operated at a single fixed location, the LAMS has been operated at a number of different locations for periods of up to a year. Its main role is as a diagnostic tool for assessing the variation in air quality around the city as a whole. It has also been deployed at several locations for specific purposes. For example, it was located at Taylor Road School for six months as part of a joint study with Leicestershire Health investigating the effects of air pollution on lung function in school children[1]. It was also deployed on Mortimer Way in the south-west of the City so as to provide information about ambient pollution levels in the area which could be used to assess the impact of a proposed power station upwind in Enderby. The LAMS was located close to the junction of Harrison Road and Gipsy Lane in the north of the City in 1997. Because of the nature of operation of the LAMS, it is not part of the AUN and real-time public access to data is not possible. However, in the future, it is likely that the LAMS will be located at "critical" locations where high air pollution levels suspected are a cause for concern[2].

4.2.3 NO_x Analysers

The AUN and LAMS monitoring stations have generally been operated in urban background locations. However, for traffic pollutants such as Nitrogen dioxide, there could be significant local variation in pollution levels around the City. The highest levels are likely to be recorded close to busy roads, but because of their size, monitoring stations are difficult to deploy at such locations. Therefore in 1997, Leicester City Council acquired two

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[1] Private communication -LCC.
[2] Private communication -LCC.

stand-alone NO_x analysers. These are very similar to those in use within the AUN and LAMS monitoring stations.

One is located on Saffron Lane where it has also been used to assess the impact of the introduction of bus lanes on pollution levels. This site could be classed as a roadside location. The second is located close to Woodgate, where it used to assess NO_x levels in an area close to a busy road and an industrial area. This site can be classed as a roadside or urban industrial location. There are also three newly installed NO_x analysers at Abbey Lane, Melton Road and Narborough Road.

4.2.4 PM_{10} Analysers

An initial assessment of data from the AUN would indicate that Ozone and PM_{10} are the pollutants giving rise to most exceedences of air quality standards. Because of the problems of long range transport of ozone pollution, local authorities are not required to consider this pollutant within their statutory review and assessment of air quality. However, there is ever-increasing concern about the health effects of PM_{10} particulates (COMEAP, 1998), and there is much uncertainty about the origin and spatial distribution of this pollutant in Leicester.

Leicester City Council established another PM_{10} analyser in the city in 1998. It is intended to monitor the worst case exposure levels, which is likely to be close to a road with very high traffic flows. The air quality standard for PM_{10} is based on a 24 hour running mean level, which means that the most appropriate location for monitoring is one where people are regularly exposed to this pollutant for long periods of time, i.e. a residential

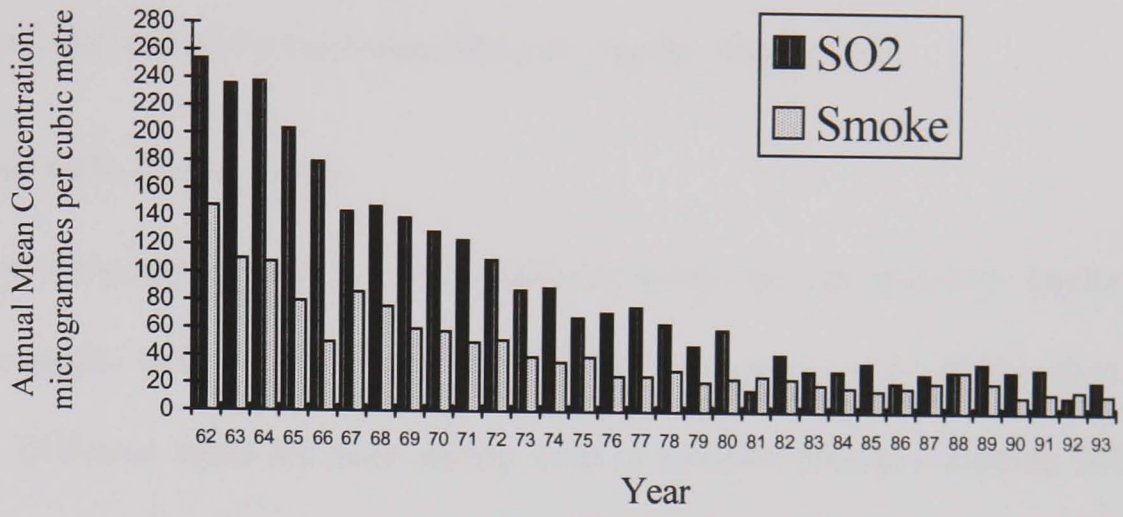
location. The exact location is therefore within the Narborough Road corridor, where some of the highest traffic flows for Leicester are recorded and where people live very close to the road (e.g. in terraced houses). It is possible that a "canyon effect" which reduces dispersion may occur for this road[3]. At Abbey Lane and Melton Road, there are two Beta Attenuation Monitors (BAM) monitors, which also measure PM_{10}. The BAM uses a different technique to the (three other) Tapered Element Oscillating Microbalance (TEOM) monitors in the city.

4.2.5 Smoke and SO_2 Monitoring Sites

The national Smoke and Sulphur dioxide monitoring networks have operated for over 30 years and have monitored the decline in the concentrations of these pollutants, resulting both from the implementation of the Clean Air Acts and from a nation-wide switch to cleaner fuels (i.e. from coal to gas). Figure 4.2 illustrates the decline in Leicester, which in the middle 1970's became one of the first cities to implement a Smoke Control Area over the whole of its area.

[3] Private communication with LCC.

Figure 4.2 Air Pollution Levels in Leicester 1962-1993



(Data source: LCC, 1994)

At its peak, the national smoke and SO_2 network included many hundreds of sites, with several in Leicester. In 1981 the network was re-organised and reduced, and currently only one Leicester site is included within the network. However, Leicester still operates two other sites, at Southfields Library and Beaumont Leys Leisure Centre, as they provide useful long-term trend data at a relatively low cost.

The monitoring system uses relatively simple technology. Daily average SO_2 levels are determined by the acid titration method (air is bubbled through Hydrogen peroxide causing the SO_2 to react to form sulphuric acid, with the pH change being measured). Daily smoke levels are determined by the reflectance method (air passing through a filter paper produces a dark stain which can be measured using a reflectometer.

Whilst smoke/suspended particulate matter and PM_{10} particulate are similar and there can be correlation between the two (APEG, 1999), they represent different fractions of

a pollutant described as "total suspended particulate". Smoke levels will include all particles above a certain size but will not take into account light-coloured particles. PM_{10} includes all particles with an aerodynamic diameter smaller than 10 mm.

4.2.6 Diffusion Tube Survey Sites

Passive sampling devices such as diffusion tubes are the cheapest method of monitoring air quality and can give a good overall picture of average pollutant levels in area (LCC, 1994). Diffusion tubes are most widely used to monitor Nitrogen dioxide, but can also be used for monitoring sulphur dioxide, hydrocarbons, ozone and ammonia.

Diffusion tubes are typically clear plastic tubes open at one end and containing a pollutant-absorbing chemical matrix or gel at the closed end. The tube absorbs the pollutant during a known exposure period (typically one week or one monthly) which is then sent to an analytical laboratory for analysis. This enables an average pollution level for the exposure period to be calculated. Because of the limited time resolution of this monitoring method, comparison with short-term air quality standards is not possible, although an estimation of compliance with longer-term standards (e.g. the annual mean standard for nitrogen dioxide) can be made.

In Leicester more than ten NO_2 diffusion tube monitoring sites have been in operation in a variety of different locations since 1992. Some of these are incorporated into national diffusion tube network, which commenced in 1993. Nationally, and locally, these are useful for identifying areas of high nitrogen dioxide concentrations (e.g. for further investigation), for determining spatial variations of pollutant levels (as a traffic pollutant,

NO_2 levels are subject to a high level of local variation), and to determine long-term trends. In Leicester, they have also been used as a low-cost method of responding to local concerns about traffic pollution levels, and therefore are often operated at some locations on a sort-term basis only.

Since 1996, Benzene diffusion tubes have been operated at three locations in Leicester. These aim to monitor levels of benzene: near a petrol filling station; at a roadside location; and, in a suburban location.

Three Ozone diffusion tube monitoring sites were established in 1997 to aid understanding of the spatial distribution of this pollutant in the City.

4.2.7 Roadside Pollution Monitors

Ten Roadside Pollution Monitors are located at roadside sites within the city. These are relatively low-cost, low precision electrochemical monitoring devices which measure nitrogen dioxide and carbon monoxide levels in heavily trafficked areas. They are primarily used for specialist research into the relationship between road traffic and air pollution (LCC, 1994).

4.2.8 Meteorological Station

In 1996, a fully automatic meteorological station was established adjacent to Groby Road on the north-western edge of the City. Because of the relation between weather conditions and pollution levels, meteorological data can assist with short-term "ad-hoc" prediction of air quality in Leicester. Also, meteorological data are an essential data input requirement for air dispersion modelling. The parameters monitored by the Leicester

Meteorological Mast include the dry-bulb temperature at 2m and 10m above ground level, the wind direction at 10m, the wind speed at 10m, the standard deviation of the horizontal wind direction and the standard deviation of the vertical wind speed. (A more detailed discussion about local meteorological data can be found in Chapter 5).

4.2.9 Description of Quality Assurance/Quality Control in Leicester

The following descriptions apply to the Leicester City Council automatic monitoring network (AUN) sites as currently operated. There is a body of historical data from the re-locatable Leicester Air Quality Monitoring Station (LAMS) which does not conform to these protocols in all respects. Also, although most deployments were for a period of typically, 3-6 months, there is a full year of data from its deployment at Rushey Mead School, Harrison Road during 1997.

Site Selection

There are seven air pollutant monitoring stations located around the City of Leicester. Six of these are fixed point stations (and includes LAMS and AUN) and one is a mobile station, which is moved around the city every 6-12 months. All of the monitoring stations contain automatic real-time analysers that produce high resolution measurements (15 minute to hourly averages). Therefore the measurements from any of these can be compared directly to the air quality standards for each pollutant.

To recap, the air pollutants monitored in Leicester are: carbon dioxide, sulphur dioxide. oxides of nitrogen and PM_{10} (particulates). The locations are a combination of urban background, roadside and suburban sites. There were selected because they were

identified as either the most likely to have air quality problem or were broadly representative of population exposure.

Equipment Selection

Even though the operating principle used to monitor each pollutant is based on the most accurate and proven analytical technique for the pollutant measured, the equipment type at each site varies (AEA, 1998). Therefore, it is important to maintain uniform operating standards and measurements methods. Accordingly, only analysers that have been tested and approved by NETCEN (the Quality Assurance/Quality Control (QA/QC) unit of the DETR) for use in the DETR Network, have been selected for Leicester. This ensures the inter-comparability of data from different sites even when the equipment type varies.

Calibration

The NO_x, SO_2, and CO analysers perform an internal automatic daily two point calibration (zero/span) to check for analyser malfunction. The zero check is made by air being passed through a chemical scrubber within the analyser to remove the pollutant Within the NO_x and SO_2 analysers, span checks are made by internal permeation tubes which release a known concentration of NO_2 and SO_2. The CO analysers do not contain an internal permeation tube. Instead, a known concentration of CO is released from a cylinder of compressed CO gas which is connected to the analyser. The ozone analysers use a UV lamp to produce ozone which is an integral part of the analyser. These daily calibrations can be checked remotely and used to identify analyser malfunction.

To check the equipment response, a manual two-point calibration is carried out fortnightly In Leicester. A zero check is made as above and a span check is made by passing

accurately predetermined concentrations of SO_2, CO, NO and NO_2 gases through the analysers from connected compressed gas cylinders (AEA, 1998). The compressed gases used are of known concentration that are traceable to National Standards.

Data Validation

The data is automatically collected (remotely via modem etc.) every day from all of the monitoring stations and checked manually. The following checks are made: that there are no unexplained gaps in the data; that there are no significant deviations in the internal daily calibrations; and that any unusual high levels are not due to instrument malfunction.

These checks ensure that only valid and reliable data are used for analysis and data loss is minimised. A high data capture rate is essential to ensure that the varying ambient conditions are represented. A record is kept of all equipment failures and data losses to determine the data capture for each monitoring site. The data capture can be used to determine the reliability of an analyser.

Data Processing Ratification

Every 1-3 months, the collected data is processed by applying the fortnightly calibration results for each analyser to its data set (AEA, 1998). The calibration results are analysed to determine whether there has been a drift in the analyser's response. If there has been a drift, this means that the analyser has been either under-reading or over-reading pollutant concentrations. The data is therefore adjusted accordingly to take account of this drift. The original raw data set is retained in case it needs to be re-examined at a later date.

The processed data is then scrutinised to check if it contains unusual or unlikely measurements, taking into account analyser history/characteristics; calibration factors/ drift;

negative or out of range data; "spikes" in data; characteristic of monitoring site: effects of meteorology; time of day/year; relationship between different pollutants and results from other sites.

Accuracy and Precision

Accuracy is defined as "the closeness of agreement between a single measured value and the actual air quality characteristic or its accepted reference value". Precision is "the closeness of agreement between mutually independent test results obtained by repeating measurement several times under stipulated conditions" (AEA, 1998). Values of the accuracy and precision of the AUN measurements were estimated by National Environmental Technology Centre (NETCEN).

As many aspects of the AUN QA/QC procedures are mirrored in Leicester's Air Quality Monitoring QA/QC procedures, the same values for the accuracy and precision have been applied to measurements made in Leicester. The estimates for the AUN (to within 2 standard deviations) are shown in Table 4.1.

Table 4.1 Accuracy and Precision of AUN data (source: AEA, 1998)

Pollutant	Accuracy (2σ)	Precision (2σ)
SO_2	$\pm$ 10%	$\pm$1.2ppb
CO	$\pm$ 8%	$\pm$0.6ppm
NO	$\pm$ 10%	$\pm$ 2.5ppb
NO_2	$\pm$ 10-11%	$\pm$ 3.5ppb
O_3	$\pm$ 11%	$\pm$ 2.0ppb
PM_{10}	Unknown	$\pm$ 4$\mu g/m^3$

Based on the above estimates, NETCEN therefore have suggested an accuracy of $\pm$ 10% as a good working figure when assessing any air quality data.

4.3. AIR QUALITY IN LEICESTER AND EAST MIDLANDS

4.3.1 Introduction of Air Quality in Leicester

Leicester is one of the largest cities in the East Midlands. Approximately 100 miles north of London, the city has access to major north-south communication routes such as canals, railways and roads. The city developed throughout the ages becoming the county's marketing centre and a base of the hosiery and textile trade.

As a result of the declaration of Smoke Control Area orders in the City (1991), oil and then gas gradually displaced coal and very little high sulphur current fuel is now used in Leicester. In July 1990, Leicester was designated Britain's first "Environment City". This was awarded by the Civic Trust and the Royal Society for Nature Conservation. As Britain's First Environment City, Leicester has an ideal opportunity to work towards sustainability using this partnership approach to deliver Leicester's Local Agenda 21. In 1990, the population of Leicester stood at 272,100 covering an area of 7,337 hectares (73.37 km^2) (LCC, 1991).

Table 4.2 shows Leicester's exceedences of National Air Quality Standards between 1994 and 1997. Air quality in Leicester is generally good in view of the small number of exceedences.

Table 4.2 Exceedences of National Air Quality Standards: Leicester AUN

Pollutant	Standard (existing 1997 strategy)	1994	1995	1996	1997
SO_2	100 ppb 15 minute mean	17 on 3 days	5 on 3 days	0	0
NO_2	150 ppb 1 hour mean	0	0	0	0
	21ppb annual mean	23ppb	23ppb	22ppb	21ppb
O_3	50ppb running 8 hour mean	75 on 12 days	192 on 26 days	120 on 16 days	126 on 19 days
PM_{10}	50µg/m3 running 24 hour mean	189 on 18 days	91 on 8 days	277 on 21 days	139 on 9 days
CO	10ppm running 8 hour mean	0	0	0	0

No exceedences for CO have been recorded from 1994 to 1997. And no exceedences are found for SO_2 in 1996 and 1997. These two pollutants are not the major concerns in Leicester. NO_2 and PM_{10} have considerable records of exceedences. The main cause of pollution in Leicester today is not industry but transport. Therefore, attention is given to traffic related pollutants and exceedences.

4.3.2 AUN Data Trends

A series of analyses of AUN data for Leicester (1994-1997) were carried out prior to the validation (Chapter 5). The first of these examines the trend in percentile levels over the period 1994 - 1997. The Pollutants examined are: SO_2, CO, NO, NO_2, NOx, O_3 and PM_{10}. The Leicester AUN data obtained from NETCEN 1994-1997 was hourly sequential. Tables 4.3-4.9 and Figures 4.3-4.9 show the Leicester annual AUN data percentile trends analysis.

AUN data percentile and trends analysis from 1994 to 1997 indicates that

- SO_2 high percentile levels from 1994 to 1997 have decreased significantly;
- Compared with 1995 and 1996, the peak level of PM_{10} in 1996 was higher than that in 1995, but the peak values of PM_{10} in 1995 was lower than in 1994. In 1997, PM_{10} values was generally lower than that in 1995 and 1996.
- The high percentile level O_3 in 1995 is the highest among the four years. This year had the highest number of exceedences (Table 4.2).

Table 4.3 Leicester SO_2 Percentile Level (ppb)

Statistic	Year 1994	Year 1995	Year 1996	Year 1997
50th percentile	5	4	3	3
84th percentile	13	12	9	7
90th percentile	16	15	11	9
95th percentile	21	20	15	13
98th percentile	28	27	21	19
99th percentile	35	35	26	25

Figure 4.3 Leicester Annual SO2 Percentile Level

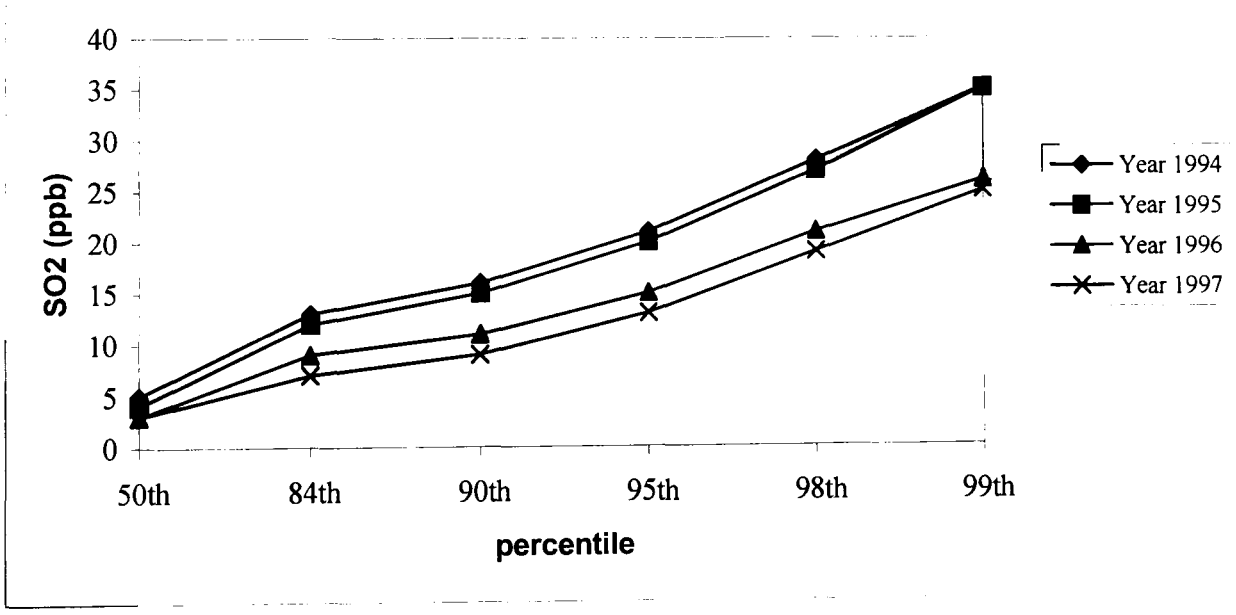


Table 4.4 Leicester PM_{10} Percentile Level ($\mu g/m^3$)

Statistic	Year 1994	Year 1995	Year 1996	Year 1997
50th percentile	18	18	18	17
84th percentile	31	30	32	30
90th percentile	37	36	38	36
95th percentile	46	44	49	44
98th percentile	57	52	66	56
99th percentile	66	59	78	64

Figure 4.4 Leicester Annual PM10 Percentile Level

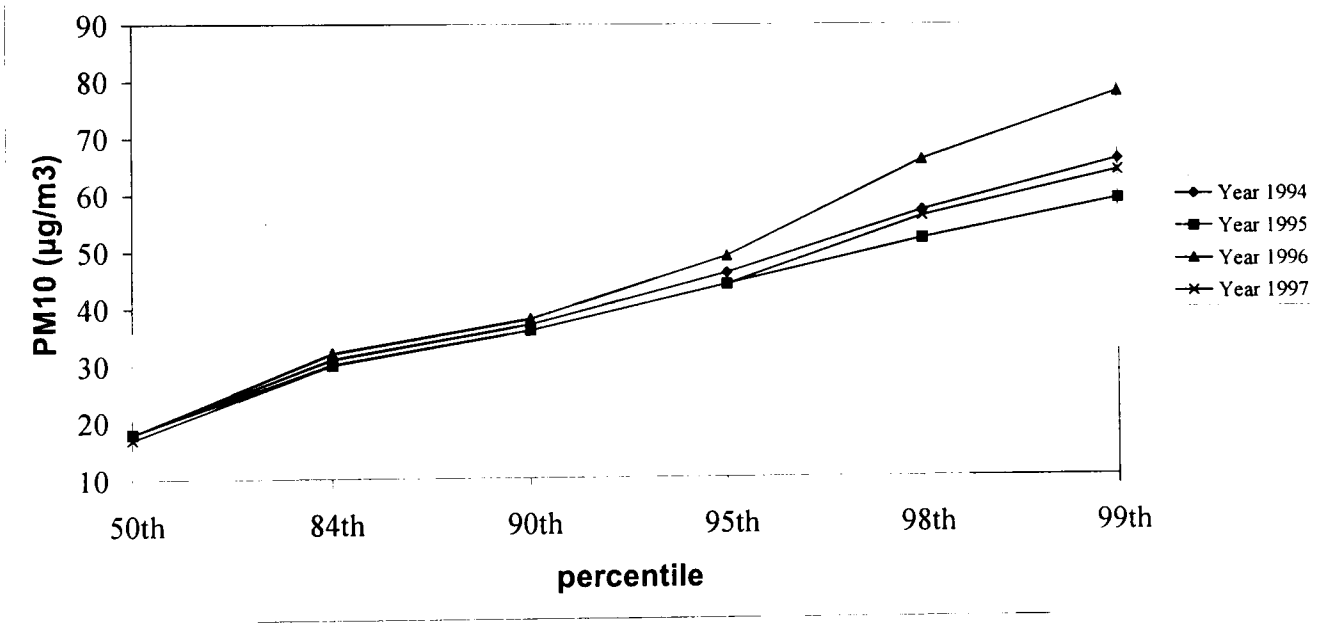


Table 4.5 Leicester NO Percentile Level (ppb)

Statistic	Year 1994	Year 1995	Year 1996	Year 1997
50th percentile	9	8	8	8
84th percentile	31	30	31	32
90th percentile	47	46	47	53
95th percentile	82	80	80	92
98th percentile	139	143	131	162
99th percentile	190	203	173	226

Figure 4.5 Leicester Annual NO Percentile Level

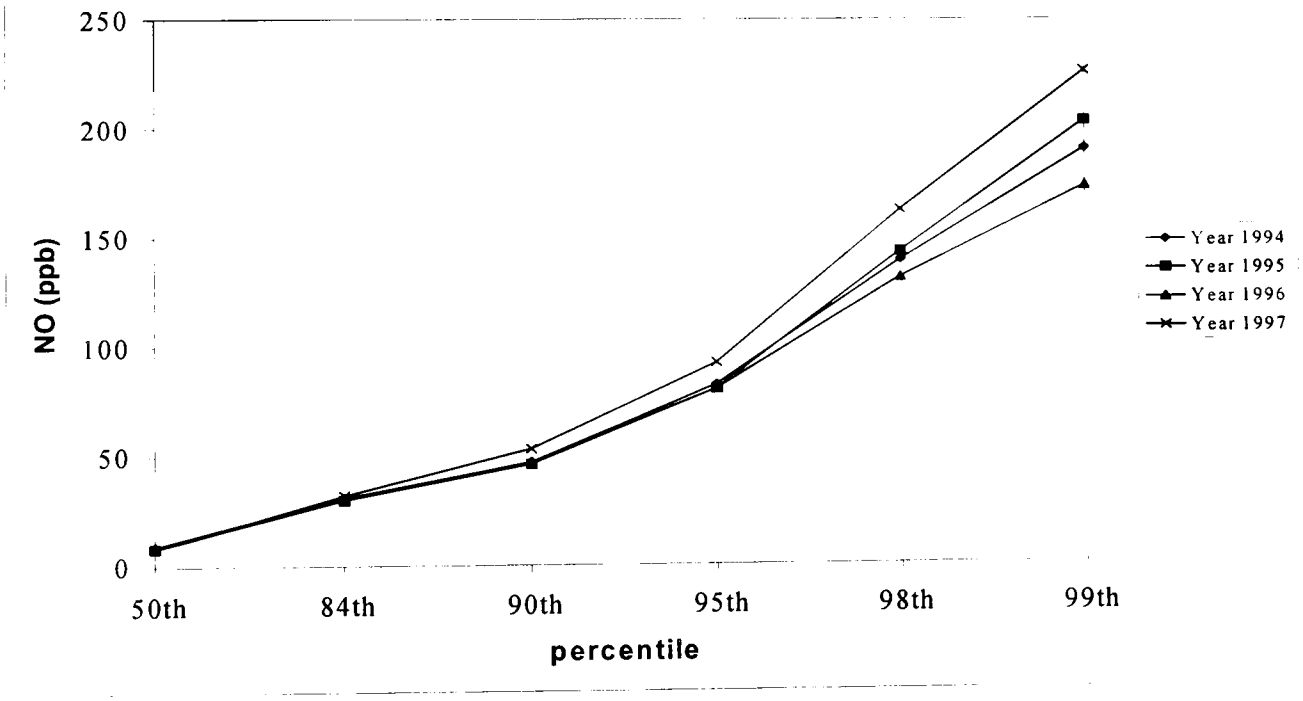


Table 4.6 Leicester NO_2 Percentile Level (ppb)

Statistic	Year 1994	Year 1995	Year 1996	Year 1997
50th percentile	22	23	22	20
84th percentile	34	34	33	32
90th percentile	37	37	36	36
95th percentile	41	42	40	41
98th percentile	47	49	46	47
99th percentile	52	55	51	54

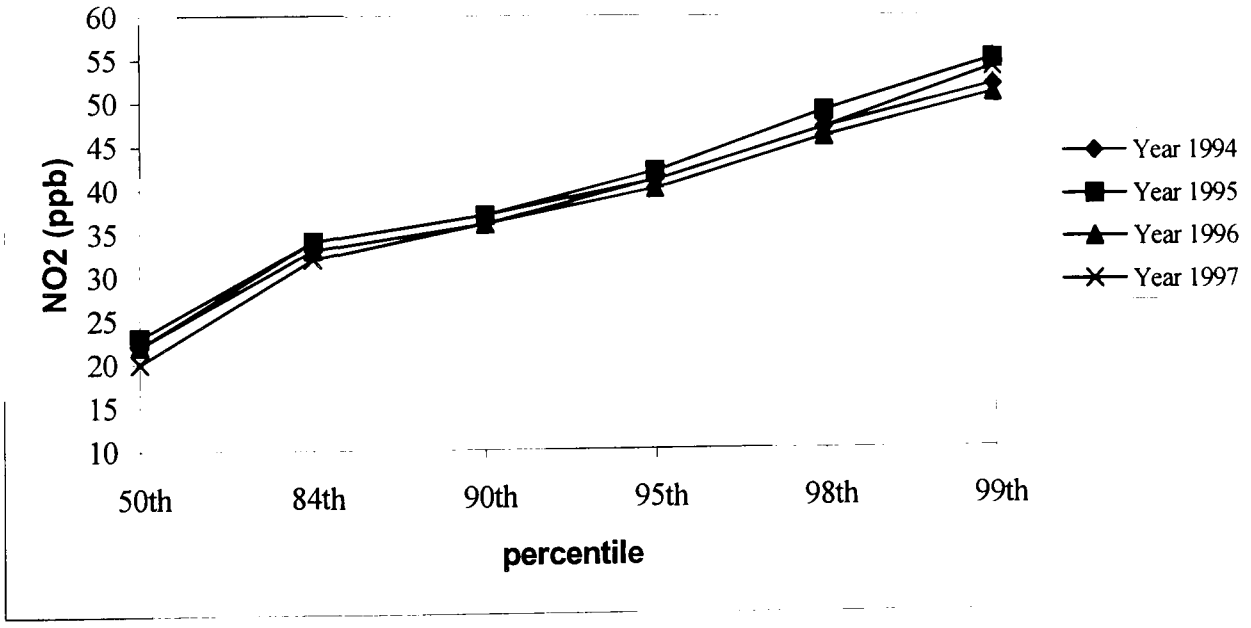


Figure 4.6 Leicester Annual NO2 Percentile Level

Table 4.7 Leicester NO_x Percentile Level (ppb)

Statistic	Year 1994	Year 1995	Year 1996	Year 1997
50th percentile	31	32	30	29
84th percentile	65	63	63	63
90th percentile	83	81	80	86
95th percentile	118	118	115	129
98th percentile	180	184	167	198
99th percentile	234	248	215	271

Figure 4.7 Leicester Annual NOx Percentile Level

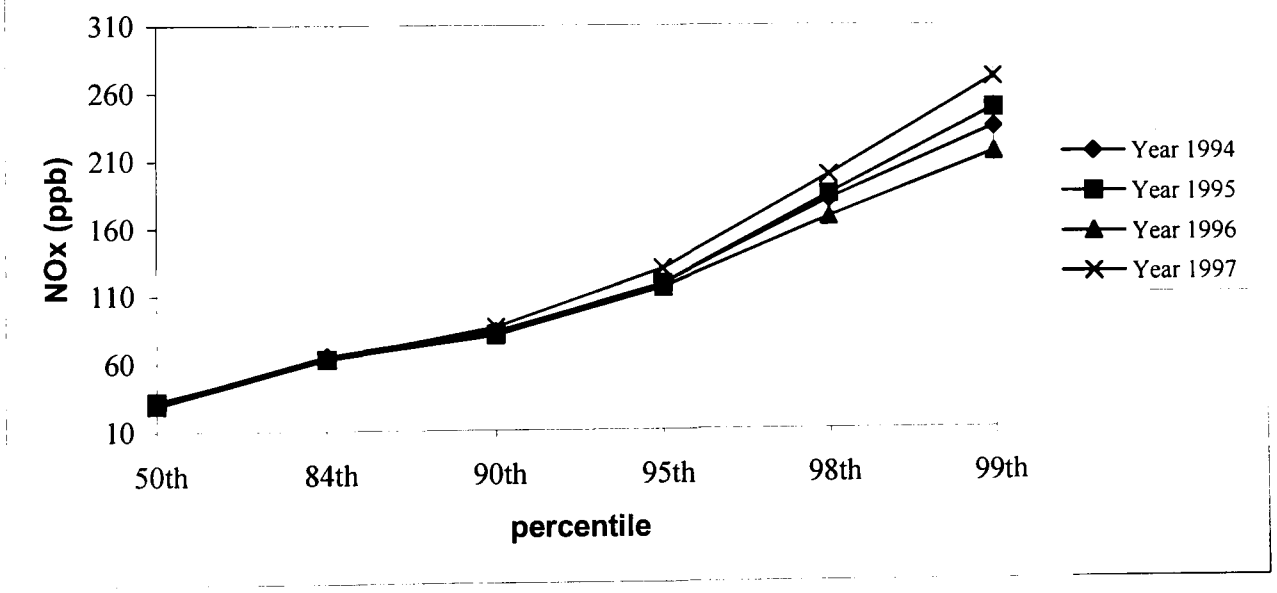


Table 4.8 Leicester CO Percentile Level (ppm)

Statistic	Year 1994	Year 1995	Year 1996	Year 1997
50th percentile	0.5	0.5	0.4	0.5
84th percentile	0.9	0.8	0.8	0.8
90th percentile	1	0.9	1	1
95th percentile	1.3	1.2	1.3	1.4
98th percentile	1.9	1.8	1.9	2
99th percentile	2.5	1.9	2.8	2.7

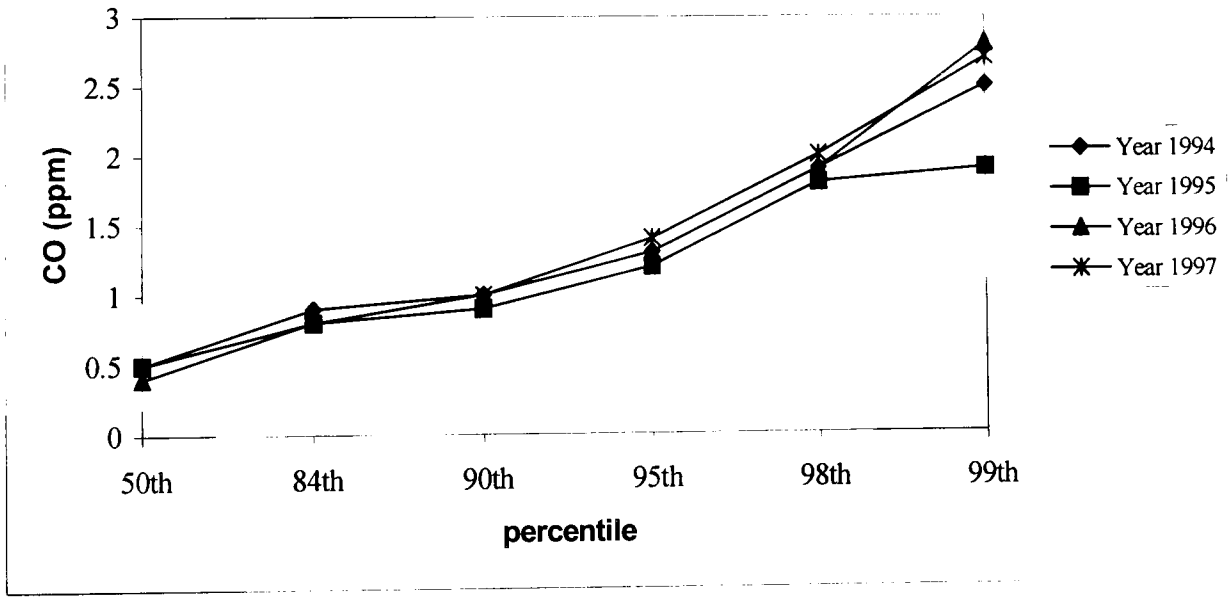


Figure 4.8 Leicester Annual CO Percentile Level

Table 4.9 Leicester O_3 Percentile Level (ppb)

Statistic	Year 1994	Year 1995	Year 1996	Year 1997
50th percentile	15	15	14	15
84th percentile	29	30	27	29
90th percentile	32	34	31	33
95th percentile	37	41	37	39
98th percentile	46	55	47	50
99th percentile	53	67	58	58

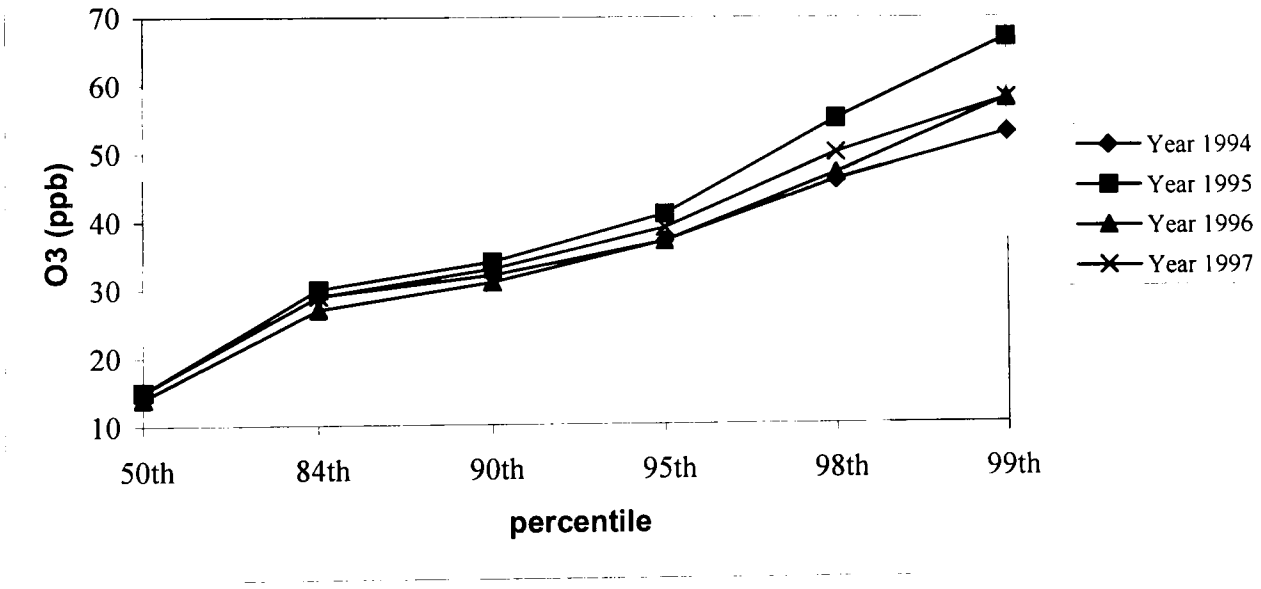


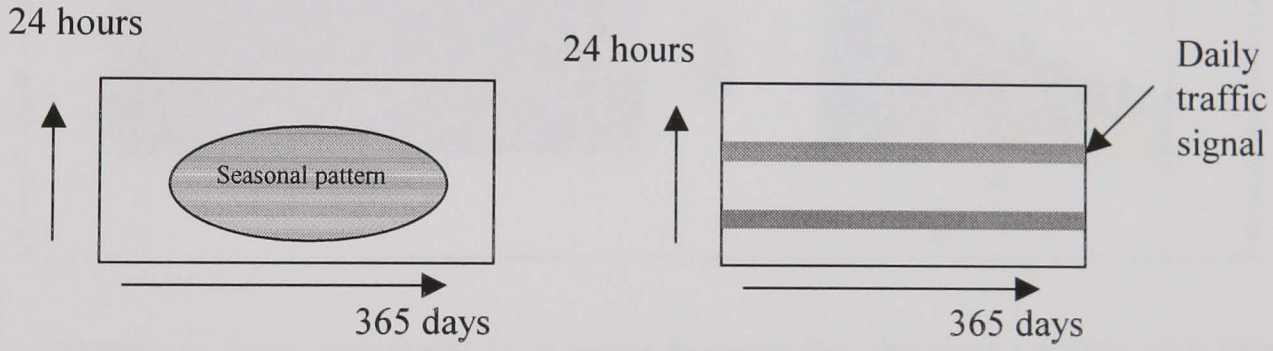
Figure 4.9 Leicester Annual O3 Percentile Level

4.3.3 Patterns in Air Quality

The software used here for the data analysis is the PV-WAVE Visual Data Analysis Software package. The programs for data analysis are written in PV-WAVE language. Programs were developed to visualise an entire year of air quality data modelled or measured using various techniques.

The AUN data for one year (8760 hourly values) are presented as: a "raw" time series; a false-colour map; and as a frequency histogram. For example, One year - 8760 values are plotted as 24 hours as y axis and 365 days as x axis, the concentration values are indicted by false-colour. Typical features that occur in annual time series for pollutants are daily and seasonal pattern (Figure 4.10).

Figure 4.10 Schematic Illustration of Air Quality Patterns

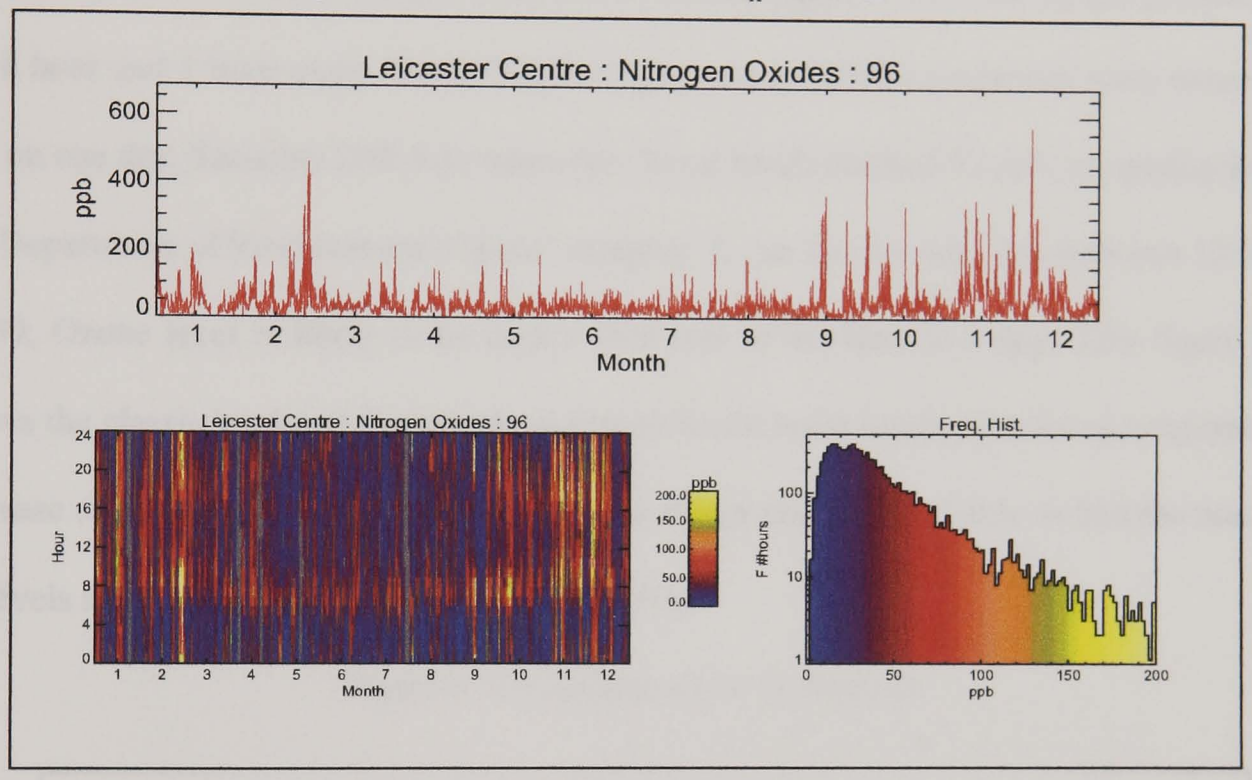


For three key pollutants - NO_x, PM_{10} and O_3, very different patterns are evident. The general air quality patterns are illustrated in Figure 4.11, Figure 4.12 and Figure 4.13. From the time series plots, the peak level can be obviously seen. From the false colour map, seasonal and daily variations can be observed, e.g., high Ozone levels often occur at summer time, in the afternoon or midday. The Frequency histogram shows how many

hours out of one year (8760 hours) the pollution concentrations are within certain levels, i.e. 40 - 41ppb, in 1 ppb bin.

Traffic patterns can be found in Figure 4.11. During traffic rush hour i.e. 8 hours -9 hours, 17 hours- 18 hours, higher level of NO_X can be seen (Figure, 4.11). Vehicular emissions are more significant, by making a greater local impact on air quality in the city, as they are emitted at ground level. It also illustrates that NO_x is mainly a winter problem.

Figure 4.11 Leicester AUN NO_x Patterns

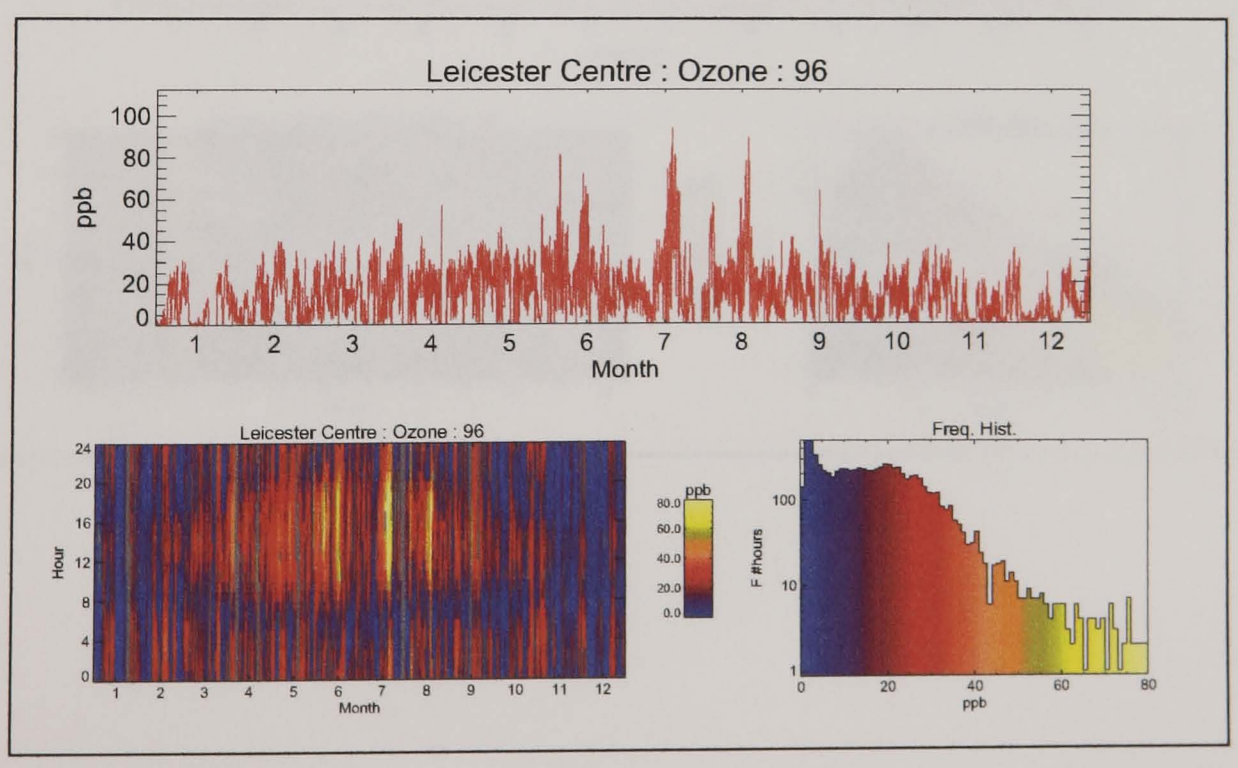


Ozone is more prominent in summer because the chemical reaction that form it depend on high levels of solar radiation. The Ozone seasonal pattern can be found in Figure 4.12. Ozone is not emitted directly from any man-made source in significant quantities. Oxides of nitrogen (NO_x) and hydrocarbons, derived mainly from man-made sources, react to form ozone. NO_x and hydrocarbons are the most important precursors of elevated levels

of Ozone. The low levels of O_3 in the morning rush hours are associated with elevated level of NOx.

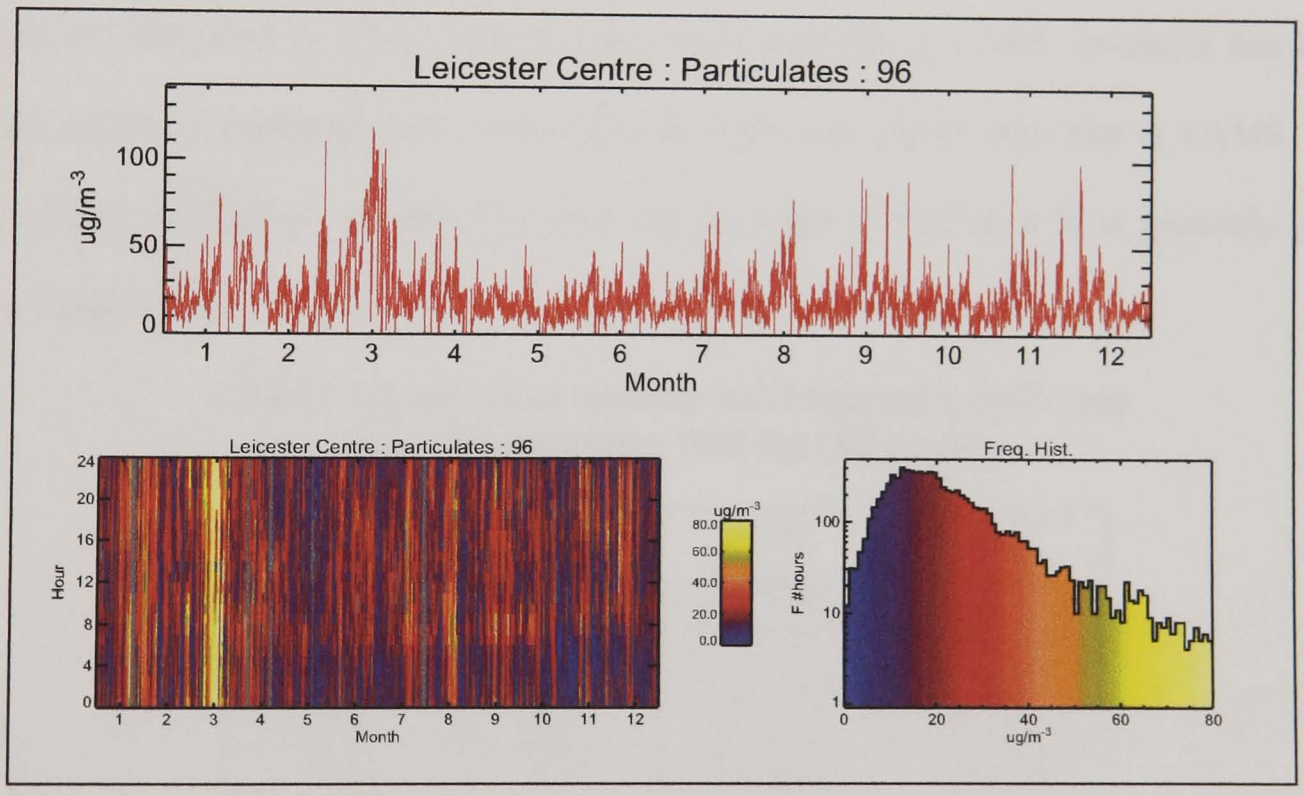
Ozone levels increase during spells of hot, calm, sunny weather. There have been problems in June-August with elevated levels of Ozone, often coinciding with periods of humid, thundery weather. However, ozone values deteriorated to 'poor' only for one or two days in one year. For example, the particularly hot and sunny spell of weather towards the end of July 1996 resulted in high levels of Ozone (see Figure 4.12). During this period both the 8 hour and 1 hour mean World Health Organisation (WHO) guidelines were exceeded, and on one day, Saturday 20th July when the Ozone levels reached 93 ppb, air quality fell to the Department of Environment's 'poor' category. It can also be seen that between 12:00 to 16:00, Ozone level is likely to be higher than rest of the time in a day. This figure also shows the classic 'peaking' that occurs as Ozone levels build during the day as temperatures increase and then fall at night when there is no longer sunlight available to fuel the reaction so levels start to disperse, a react with NO to NO_2.

Figure 4.12 Leicester AUN O_3 Patterns



Unlike NO_x and O_3, the pattern for the particulates (PM_{10}) does not show any obvious relation to the day or to the seasons. However, there is faint evidence of a traffic signal in the morning. Unlike the gaseous pollutants, particulate matter in the atmosphere is composed of a wide range of materials arising from a variety of sources. Over the last two years, a growing body of evidence has suggested that remote i.e. imported pollution sources play a major role in determining PM_{10} concentrations, even in urban areas. This view could also be reflected in Figure 4.13, because no clear seasonal or traffic pattern can be seen. It does show the episodic nature of PM_{10} problems. A big episode in March (months) lasted several days, but little or no variations were shown during the day. Peak levels of PM_{10} are often related to a specific meteorological condition.

Figure 4.13 Leicester AUN PM_{10} Patterns



4.3.4 AUN and LAMS Comparison

The comparisons between AUN and LAMS data were carried out to exam if there are any air pollution level similarities or variations across the city. This is also a part of preparation for the validation of ADMS_Urban.

LAMS data was collected in Mortimer Way from July 1996 to December 1996. The comparison was undertaken with Leicester AUN data at the same period from July 1996 to December 1996. The correlation between these two sites for various pollutants is shown in Table 5.2 and 5.3. The pollutants compared were: SO_2, CO, NO, NO_2, NOx, O_3 and PM_{10}.

The percentile plots (see Figure 4.14) show that, in the main, AUN and LAMS data agreed well. Some "steps" were appeared in AUN percentile lines (Figure 4.14), this is because AUN data were ratified first then made available by NETCEN (as noted earlier). However, SO_2 level at AUN was noticeably lower than that at LAMS (evidence that local point source is presented later). NO_2 level at AUN was higher than that at LAMS. The correlation coefficient between these two sites of order of 0.61 to 0.92 is generally good (see Table 4.10).

Table 4.10 Comparison between AUN data and LAMS Data
July 1996-December 1996 (by half a year)

Pollutants	Correlation coefficient	AUN Average	LAMS Average
CO	0.61	0.666 ppm	0.594 ppm
NO	0.82	23.3 ppb	28.5 ppb
NO_2	0.71	20.3 ppb	16.1 ppb
NO_x	0.83	44.1 ppb	45.4 ppb
O_3	0.92	14.6 ppb	12.6 ppb
PM_{10}	0.87	19.6 $\mu g/m^3$	23.0 $\mu g/m^3$
SO_2	0.68	4.81 ppb	3.60 ppb

The following are noted:

- AUN and LAMS correlated with a high degree of coefficient.
- The highest correlation was for Ozone.
- There was a greater variation of coefficient for CO and NO_2 than that for the ozone between AUN and LAMS sites. This suggests the importance of the local traffic effects to the levels of CO and NO_2.

In summary, air quality in Leicester is general good. The traffic related pollutants cause the major public concern, and the pollution levels vary across the city depending on traffic conditions and locations.

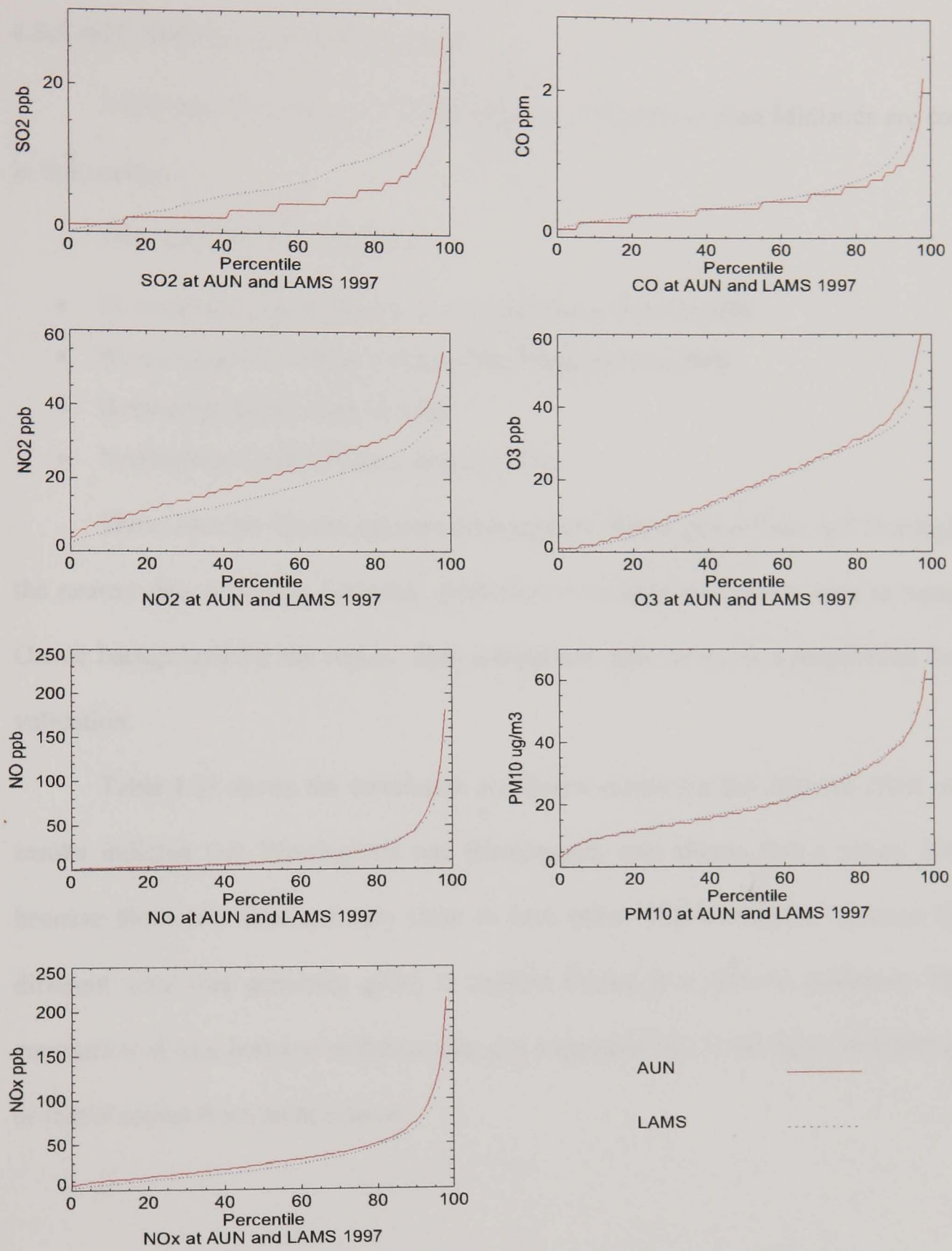


Figure 4.14 AUN and LAMS Data Percentile Analysis

4.3.5 AUN Data for the East Midlands

AUN data for Leicester and four other nearby cities in East Midlands are compared in this section.

The other four AUN sites were:

- Birmingham centre (Birm.), data period from 1994 to 1996
- Birmingham East (BirE.), data period from 1994 to 1996
- Bottesford (Bott.), data in 1996
- Nottingham Centre (Nott.), data in 1996

These sites are chosen because Birmingham, Birmingham East, and Nottingham are the nearest data sets from Leicester. Bottesford is a rural area and is used to measure the Ozone background for the region. This comparison also serves as a preparation for model validation.

Table 4.11 shows the correlation coefficient matrix for the different AUN sites. The results indicted that Birmingham and Birmingham east always had a strong correlation because these two sites are very close to each other. The correlation between Ozone at different sites was generally good; it implied Ozone is a national pollutant. The weak correlation of SO_2 between different data sets suggested SO_2 is the more localised pollutant or that if comes from point sources.

Table 4.11 Correlation Coefficient between AUN Different Data Sets

		Birm	BirE	Bott	Leic	Nott
CO:1994	Birm	1	0.71	n/a	0.58	n/a
	BirE	*	1	n/a	0.65	n/a
	Bott	*	*	1	n/a	n/a
	Leic	*	*	*	1	n/a
	Nott	*	*	*	*	1
NO_2: 1994	Birm	1	0.82	n/a	0.61	n/a
	BirE	*	1	n/a	0.71	n/a
	Bott	*	*	1	n/a	n/a
	Leic	*	*	*	1	n/a
	Nott	*	*	*	*	1
NO: 1994	Birm	1	0.77	n/a	0.67	n/a
	BirE	*	1	n/a	0.79	n/a
	Bott	*	*	1	n/a	n/a
	Leic	*	*	*	1	n/a
	Nott	*	*	*	*	1
NOx: 1994	Birm	1	0.79	n/a	0.68	n/a
	BirE	*	1	n/a	0.79	n/a
	Bott	*	*	1	n/a	n/a
	Leic	*	*	*	1	n/a
	Nott	*	*	*	*	1
O_3: 1994	Birm	1	0.9	0.66	0.72	n/a
	BirE	*	1	0.77	0.82	n/a
	Bott	*	*	1	0.8	n/a
	Leic	*	*	*	1	n/a
	Nott	*	*	*	*	1
PM_{10}: 1994	Birm	1	0.8	n/a	0.73	n/a
	BirE	*	1	n/a	0.71	n/a
	Bott	*	*	1	n/a	n/a
	Leic	*	*	*	1	n/a
	Nott	*	*	*	*	1

Table 4.11 Correlation Coefficient between Different AUN Data Sets (continued)

SO_2:1994	Birm	1	0.75	n/a	0.38	n/a
	BirE	*	1	n/a	0.37	n/a
	Bott	*	*	1	n/a	n/a
	Leic	*	*	*	1	n/a
	Nott	*	*	*	*	1
CO:1995	Birm	1	0.66	n/a	0.56	n/a
	BirE	*	1	n/a	0.63	n/a
	Bott	*	*	1	n/a	n/a
	Leic	*	*	*	1	n/a
	Nott	*	*	*	*	1
NO_2:1995	Birm	1	0.85	n/a	0.62	n/a
	BirE	*	1	n/a	0.7	n/a
	Bott	*	*	1	n/a	n/a
	Leic	*	*	*	1	n/a
	Nott	*	*	*	*	1
NO: 1995	Birm	1	0.83	n/a	0.73	n/a
	BirE	*	1	n/a	0.8	n/a
	Bott	*	*	1	n/a	n/a
	Leic	*	*	*	1	n/a
	Nott	*	*	*	*	1
NO_x: 1995	Birm	1	0.85	n/a	0.74	n/a
	BirE	*	1	n/a	0.8	n/a
	Bott	*	*	1	n/a	n/a
	Leic	*	*	*	1	n/a
	Nott	*	*	*	*	1
O_3: 1995	Birm	1	0.91	0.69	0.78	n/a
	BirE	*	1	0.78	0.85	n/a
	Bott	*	*	1	0.81	n/a
	Leic	*	*	*	1	n/a
	Nott	*	*	*	*	1

Table 4.11 Correlation Coefficient between Different AUN Data Sets (continued)

PM_{10}: 1995	Birm	1	0.78	n/a	0.69	n/a
	BirE	*	1	n/a	0.63	n/a
	Bott	*	*	1	n/a	n/a
	Leic	*	*	*	1	n/a
	Nott	*	*	*	*	1
SO_2:1995	Birm	1	0.82	n/a	0.4	n/a
	BirE	*	1	n/a	0.39	n/a
	Bott	*	*	1	n/a	n/a
	Leic	*	*	*	1	n/a
	Nott	*	*	*	*	1
CO:1996	Birm	1	0.61	n/a	0.45	0.63
	BirE	*	1	n/a	0.54	0.55
	Bott	*	*	1	n/a	n/a
	Leic	*	*	*	1	0.61
	Nott	*	*	*	*	1
NO_2:1996	Birm	1	0.81	n/a	0.59	0.7
	BirE	*	1	n/a	0.67	0.72
	Bott	*	*	1	n/a	n/a
	Leic	*	*	*	1	0.8
	Nott	*	*	*	*	1
NO: 1996	Birm	1	0.76	n/a	0.57	0.59
	BirE	*	1	n/a	0.68	0.63
	Bott	*	*	1	n/a	n/a
	Leic	*	*	*	1	0.7
	Nott	*	*	*	*	1

Table 4.11 Correlation Coefficient between Different AUN Data Sets (continued)

NOx: 1996	Birm	1	0.78	n/a	0.6	0.64
	BirE	*	1	n/a	0.7	0.66
	Bott	*	*	1	n/a	n/a
	Leic	*	*	*	1	0.73
	Nott	*	*	*	*	1
O_3: 1996	Birm	1	0.91	0.71	0.76	0.73
	BirE	*	1	0.82	0.84	0.81
	Bott	*	*	1	0.84	0.8
	Leic	*	*	*	1	0.89
	Nott	*	*	*	*	1
PM_{10}: 1996	Birm	1	0.9	n/a	0.77	0.59
	BirE	*	1	n/a	0.8	0.66
	Bott	*	*	1	n/a	n/a
	Leic	*	*	*	1	0.75
	Nott	*	*	*	*	1
SO_2:1996	Birm	1	0.76	n/a	0.43	0.45
	BirE	*	1	n/a	0.4	0.36
	Bott	*	*	1	n/a	n/a
	Leic	*	*	*	1	0.53
	Nott	*	*	*	*	1

4.4 CONSTRUCTION OF THE LEICESTER EMISSION INVENTORY FOR ADMS_URBAN

An air pollution emissions inventory is a compilation of the sources of an air pollutant or pollutants within a particular geographical area. The inventory usually includes information on the amount of the pollutant released from major industrial sources, average figures for the emissions from smaller sources, and from transport throughout the area. Emission inventories are an essential tool in the management of local air quality. Emission inventories identify the sources enable modelling of air quality and help in preparing abatement strategies, whilst air quality monitoring, such as that carried out through the UK Automatic Urban Networks (AUN), shows the concentration of air pollution at various sites in the UK.

By identifying the sources of air pollutants, an atmospheric emissions inventory can be used as an aid in interpreting air quality measurements. There are four recognised forms in which data is stored in an inventory. Air pollution is generally described as being from either a point source, a line (i.e. transport) source, an area source and a grid source.

4.4.1 Characterisation of Emission Inventory

Point Sources

A point source is one whereby pollution is emitted from within a limited geographical area that can be identified by way of a specific map reference, such as an industrial site. The pollutants may be emitted from a building or chimney, or from several

emission points near to the referenced point source. The industrial processes were designated by the Regulations (Environmental Protection Act 1990) as prescribed Part A or Part B processes depending on their polluting potential. The prescribed processes were those identified as having the potential to release into the air significant quantities of prescribed pollutants. For those with the greater potential to pollute are Part A processes. authorisation and legislative control of such processes is the duty of the Environment Agency. Part B processes generally have less polluting potential; authorisation and legislative control of these processes is the duty of the local authority (Buckingham, et al., 1997). Many such processes may be required to maintain an inventory of their emissions.

Line sources

Line sources include emissions from road, rail and air transport. For urban areas, it is generally the case that only roads are considered.

Area Sources

An area source contains numerous point sources each emitting relatively small quantities of pollution. Taken on its own, each individual source within the area would be considered to be insignificant and not worthy of individual identification; however, when the pollution from many sources is considered, the accumulation of all the numerous emissions contribute sufficiently to the background air quality to be significant. For example, a commercial centre containing many businesses or shops, or a large residential area, may contain sufficient sources to warrant being described as an area source due to the emissions from central heating boilers.

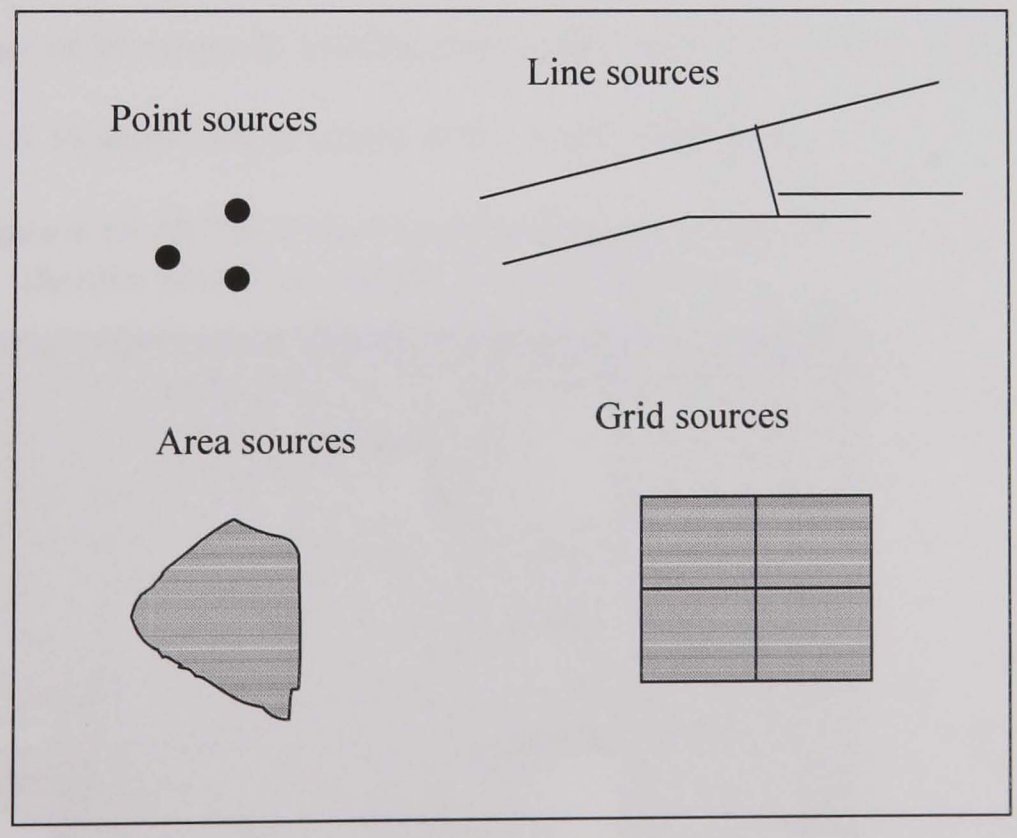
Grid Sources

Grid sources mean background emission levels from a variety of small sources that are combined into a 1km x 1km grid, for example emissions from households. Points and line sources can be super-posed on or across area and grid sources.

Atmospheric inventories are an essential tool in the management of local air quality. They allow the user to examine the geographical distribution of pollutants across a region. They also allow the assessment of the relative significance of different sources of air pollution, for example, the proportion of carbon monoxide emissions in a district arising from vehicular emissions, and help in planning abatement strategies.

A simple illustration of point source, line source, are source and grid source is shown in Figure 4.15.

Figure 4.15 Schematic Illustration of Various Sources



4.4.2 ADMS_Urban Emission Inventory

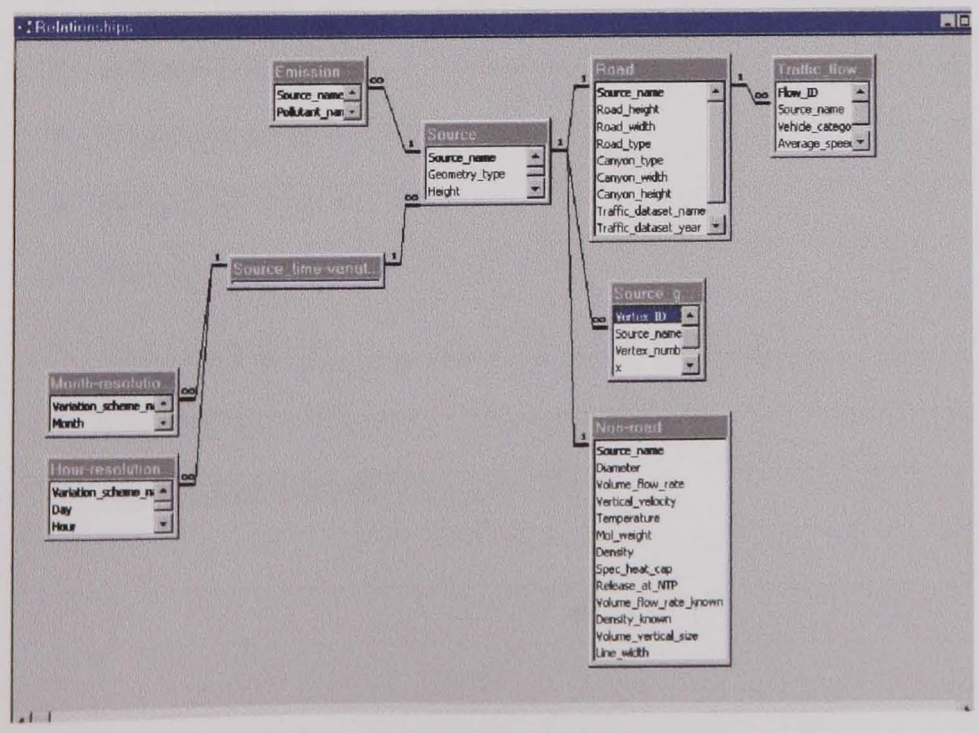
ADMS_Urban has structures designed specifically to store the available knowledge about ambient air emission sources within its software framework. ADMS_Urban can access directly an emission inventory database which contains some or all of the following data in brief:

- Source location, height, geometry (non-road sources) or road geometry, width and height of adjacent buildings (road sources)
- Pollutant name, emission rate
- Monthly or hourly variation of emission rate
- Vehicle type, count and average speed (road sources) or emission data e.g. Specific heat capacity, volume flow rate (non-road sources)

The ADMS_Urban emissions inventory is in the form of a Microsoft Access database that is linked to Geographic Information System (GIS) ArcView. Data can either be input into Access by copying and pasting data for groups of sources from a spreadsheet package or by manually entering information source by source directly into ADMS_Urban.

Figure 4.16 shows the structure of the emission database.

Figure 4.16 ADMS-Urban emission database structure
(Screen Shot from ADMS_Urban Interface)



4.4.3 Construction of the Leicester Emission Inventory

The purpose of the Leicester Atmospheric Emissions Inventory is as follows:

- as an input to local policy-making with respect to pollution abatement and control;
- to assist in judging the effectiveness of existing policies;
- as an aid to the interpretation of air quality measurements;
- as an input to atmospheric dispersion models; and,
- for general public information.

With respect to the data requirement of ADMS_Urban, the construction of Leicester emission inventory is discussed in the following.

Point sources

Specific information was provided on those industrial processes which have been authorised under Part 1 of the Environmental Protection Act 1990 and of boiler plants with a capacity greater than 2 megawatt hours. The emission inventory used in this study listed 199 point sources including part A processes, part B processes and boiler plants in Leicester. The following data for each source was provided:

- Name of the source
- Process type
- Various pollutants for each source (pllutant name)
- Annual emissions of various pollutants for each source (Emission rate (g/s))
- Location of the sources
- Height of chimney (m)
- Inner diameter of chimney (m)
- Vertical velocity of release at source exit (m/s)
- Volume flow rate (m^3/s) (otional item)
- Temperature of the release (°C)

- Time varying factors (e.g. diurnal or season variation in emissions)

Processes could be assumed to operate 24 hours a day 365 days a year, no variation. The emission database in Leicester comprised 52 Part A and Part B point sources and 4 power station/ plants point sources outside of Leicester boundary.

Line Sources (Road sources)

For the Leicester emission inventory used in Leicester, traffic flows were taken from runs of the Greater Leicester Traffic Model (GLTM), which is based on the TRIPS (Transport Planning Software) Model. These were performed by the Planning and Transportation Department of Leicestershire County Council for its area as constituted prior to Leicester City Council achieving Unitary Status on 1st April 1997.

The TRIPS Model is designed to calculate traffic flow from land-use factors such as population, housing, industrial activity etc. The model also takes account of physical characteristics of roads such as carriageway widths and speed limits.

For the purposes of the TRIPS Model, roads are separated into "links", i.e. straight lengths of road between significant junctions. The TRIPS Model uses data on around 3,500 links for the area covered by the pre-Unitary Status County of Leicestershire (LCC, 1999). Each link has an identifying number and spatial co-ordinates fixing either end of the section of road concerned. The percentage of heavy and light vehicles using a particular road is calculated from the road type. Hourly averages are then calculated for the heavy and light vehicle categories. Road width is standardised according to the number of lanes across the particular carriageway. For each road link, the Model outputs morning peak, evening peak and off-peak flow and speed data.

Clearly one cannot calculate pollutant emissions for vehicles from traffic counts alone. Furthermore, a breakdown of the vehicle types, travelling along each road link, was not available. However, general information was supplied about the composition of the vehicles for three different road-types, A-roads, B-roads and unclassified roads, and this relationship is assumed to be constant both through time of day and day of week. The composition for the appropriate road type was applied to each road link in the inventory.

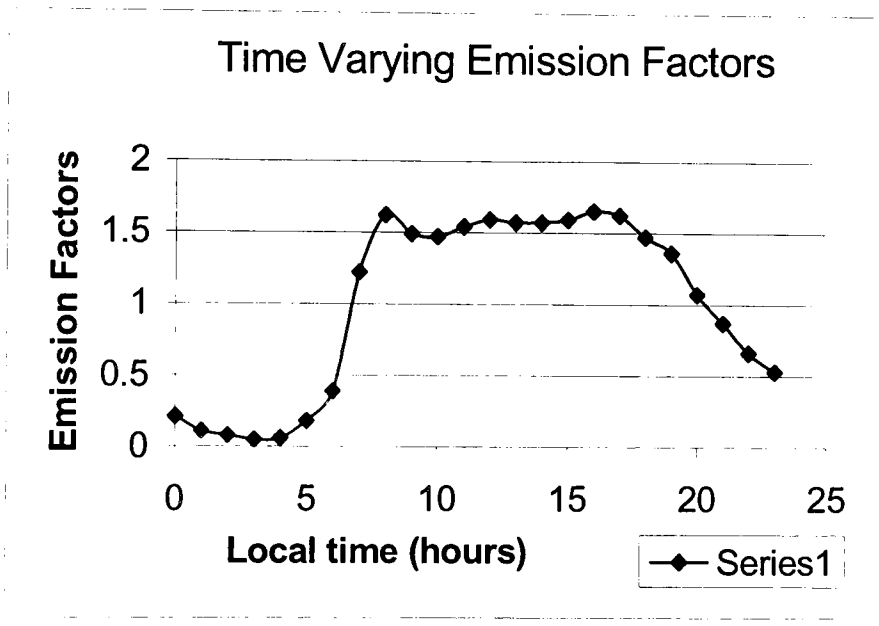
Emission factors were supplied for different vehicle types and many of these contained factors that varied with speed, which is contained in the model ADMS_Urban. Emission rate of pollutants are calculated from traffic flow data: vehicle type (whether heavy duty or light duty), vehicle average speed and vehicle count i.e. the number of vehicles per hour passing along a stretch of road in unit time. The emission rates are in kg/m/s for CO, CO_2, NO_x, hydrocarbons and particulate. The input parameters for road sources are as follows:

- The type of road for each link (e.g. motor way, A road etc.).
- Length of link, a start and end grid co-ordinates.
- Total vehicles per day along each link.
- Hourly variations along each link (numbers/hr).
- Average speed of vehicles on road links (km/hr) (to the nearest 10km/hr).
- Split between heavy and light vehicles for different road types.
- Two-way traffic flow as well as a traffic flow each way (i.e. A to B, and B to A).
- Vehicles emission factors at different speeds for heavy and light vehicles (Various pollutant, (g/km)), emission rate of various pollutants (g/km/s).
- Road width (m).
- Canyon height (m).

- Elevation of road (m).
- Time varying emission factors (Variation in times and day of week traffic number).

Time variation factor is to reflect the different traffic flow patterns over a day, i.e. traffic peak hours (7hours -9 hours, 16 hours - 18 hours), or less traffic period (1am -5am) etc. Figure 4.17 shows the daily traffic time varying emission factor applied in ADMS_Urban model. There are small peaks for morning and afternoon rush hour traffic over a fairly constant level from 8 hours to 18 hours.

Figure 4.17 Time Varying Emission Factors in ADMS_Urban



Area sources

Except for industry chimney and road sources, many sources could be described as area sources, i.e. emissions from residential areas. ArcView (a Geographical Information System (GIS) package) is used to define areas. The unit of input emission rate is g/ m^2 /s. There are total 12 area sources in Leicester's emission database, mainly for residential areas.

Grid Sources

As ADMS_Urban version 1.51 had a fixed limit of 1500 sources. With the large number of line, points and area sources in Leicester, sources need to be selected carefully. After the top 1200 sources were selected, the remaining sources were aggregated to 1km x 1km grid squares covering the whole of Leicester for the purpose of modelling. Each grid square contains the following layers of information:

- Major Roads - Emissions from the main roads network
- Minor Roads - Emissions from minor roads
- Part A&B - Emissions from part A and B processes

Summary of Leicester Emission Totals

The emission totals for different pollutants in Leicester emission database are summarised in Table 4.12. It shows that the major contributions of pollution are from traffic road sources but not from industrial point sources in Leicester.

Table 4.12 Industry and Transport Emissions in Leicester (tonnes/year, 1997)

Pollutants	Industry emissions	Road transport emissions	Area Sources	Emissions Total	Industry % of total emissions	Road transport % of total emissions
CO	18.8	43946.8	7.0	43972.6	0.1	99.9
NO_2	n/a	416.0	n/a	416.0	n/a	100
NO_x	154.1	12558.2	135.8	12848.1	1.2	97.7
PM_{10} [1]	n/a	414.3	n/a	414.3	n/a	100
SO_2	125.6	0	0	125.6	100	0

1. Note: Only primary sources of PM_{10} are contained in the emission database. More detailed discussion of other sources of PM_{10} (coarse and imported matters) can be found in section 5.4.2.

Ordnance Survey (OS) data

Local OS data is required to display the location of the emission sources and, after modelling, their dispersal patterns. The data may be entered via a GIS (Geographical Information System), from an emissions inventory database in a standard database package or via ADMS_Urban windows interface. The GIS, displays a map of the source area at a variety scales. With the map on the screen the user can define the location of sources and the area over which results should be calculated.

4.4.4 Limitations of Leicester Inventory

The emissions inventory contains many assumptions and approximations. For example, the details of the emissions from the industrial plant are taken from the application documents and represent a worst case scenario, i.e. the plant emitting its maximum permitted amount for all hours of operation. Clearly this will not be the case for the majority of the time, and hence an error is introduced here.

The vehicle count information is considered to be relatively accurate even though much of it has been derived from a traffic model. Emissions for motor vehicles contribute a high proportion of the emission of several pollutants. Accurate vehicle emission factors are therefore essential if one is to assess air quality. Vehicle emission factors are constantly being revised as the methods used to measure these emissions improve. The speed of traffic has a great bearing on the amount of pollution produced by each road link (LCC, 1999). Similarly, more accurate estimates need to be made on the average vehicle speed on a particular road and the variability with the time of day and day of the week. More

information about the vehicle type composition on individual road links at different times of the day, day of week and month of the year are needed.

Leicester is situated on the Midland main railway line from London St. Pancras to Sheffield and the North. Two subsidiary routes, running towards Coalville and Nuneaton make junctions with the main north-south route within or near the City boundary, at Knighton and Wigston Junctions, respectively. Information for rail sources are often dealt with as individual line sources too, but in this inventory the information was not available. For the purposes of this study, emissions from rail traffic have been treated as negligible and have not been included in the emissions inventory used as input to the dispersion models.

The grid source data used in the Leicester Emissions Inventory are aggregated. For example, following the selection of major point sources and road sources, the rest of the sources (both points and road sources) are aggregated to grid sources. As with the point and line sources more accurate time-varying emission factors may need to be applied to each grid layer. However, there are no time variation factors being applied to grid sources. These limitations in emission inventory need to be treated with caution. It should be noted that dispersion models are only as good as the underlying emission inventories.

CHAPTER 5 APPLICATION OF ADMS_URBAN - VALIDATION I

5.1 INTRODUCTION

In this Chapter, target validation data sets and the meteorological data for modelling are presented first. A description of the validation methodologies used for this study then follows. The model used here is ADMS_Urban version 1.51, the latest version released by Cambridge Environmental Research Consultants Ltd. (CERC) at the end of 1998. The results of validation tests for the ADMS_Urban model and the overall performance of the model are the major part of this chapter.

The validation test is based on the model's ability to reproduce pollution levels that were measured in Leicester between 1994 and 1997. The prediction of past events is referred to here as a "hindcast". Several "hindcast" scenarios were simulated for the pollutants CO, NO_2, NO_x and PM_{10}. Annual ADMS_Urban predictions using Elmdon meteorological data for the entire year from 1994 to October 1997 were carried out. The purpose of annual runs was to compare the percentile lines for the measured and modelled pollutants.

In addition to these, hourly predictions of pollution levels for the pollutants CO, NO_2, NO_x and PM_{10} for selected summer and winter of episode weeks and non-episode periods were also made. An "episode" is the high pollution levels persist for a few days. The summer and winter periods chosen were June 1994, December 1994, June 1995, and November 1995. The episode periods were August 1996, December 1996, and January

1997. Percentile analysis of the ADMS_Urban output, compared with AUN monitored data were carried out for each pollutant. Time series comparison was also carried out for the selected periods. The comparison of modelled and measured data was undertaken in the PV-WAVE programming environment. Details of model runs are shown in Appendix B, where details can be found of the name of model scenario, the emission database used and the meteorological data used etc.

5.2 ADMS_URBAN VALIDATION: PREPARATION

5.2.1 Target Data Sets

The Leicester AUN monitoring station contains automatic analysers calibrated to a high standard which measure oxides of nitrogen (NO and NO_2), sulphur dioxide, carbon monoxide, PM_{10} and ozone. Throughout the UK, each monitoring station in the AUN network utilises instruments which sample and analyse the ambient air continuously (AUN data are available to public via web site http://www.aeat.co.uk/netcen/airqual/index.html). As noted earlier, UK air pollutant measurements are based on a rigorous quality assurance and control programme, and utilise traceable and cross-checked calibration chains. Gas standards and procedures are regularly checked and inter-compared on an international scale (Chapter 4, section 4.21). A recent exercise involved a series of WHO workshops that demonstrated UK measurement standards to be within 5% of corresponding Europe-wide standards for NO_x , SO_2, and CO and within 2% for O_3 (AEA, 1998). Instruments currently deployed in Department of Environment and Regions (DETR) automatic monitoring networks use the following measurement techniques (see Table 5.1).

Table5.1 Measurement Technique in AUN

Pollutant	**Measurement Technique**
Ozone	UV absorption
Oxides of Nitrogen	Chemiluminescence
Carbon Monoxide	IR absorption
Sulphur Dioxide	UV fluorescence
PM_{10}	Tapered Element Oscillating Microbalance
Hydrocarbons	Gas chromatography

AUN data is the longest and high-quality continuous monitored data set available for Leicester. The AUN station in Leicester is located within the urban centre, approx. 30 metres from the nearest major road. Comparison of ADMS_Urban predictions for a range of pollutants outputs with AUN monitored data is one of the principal means for model validation. The target data sets used for the validation also include the LAMS data, NO_x roadside analyser data and additional PM_{10} monitoring data.

5.2.2 Emission Database

The emission database for Leicester comprises 1496 sources, which is just below the 1500 sources limitation of current ADMS_Urban model. Most of the point sources and some road sources were aggregated to grid sources to reduce whole number of sources being taken into simulation, the other parts of the emission database contains the rest of the major road sources and some large point sources in Leicester (See Figure5.1). The emission database contains emission values for pollutants CO, NO_2, NO_x, PM_{10}. Therefore, the general performance is based on the scenario runs for these pollutants. Leicester's SO_2 emissions are primarily from relatively minor point sources. For practical reasons, a

emission database for SO_2 was constructed from these point sources. Therefore, the predicted SO_2 values are produced in the different scenario runs. From the analysis in the Chapter 4, we can see that CO and SO_2 rarely cause exceedences, and they are not considered to be a major concern in this study. The modelling in this study is focused on the key pollutants: NO_2, NO_x and PM_{10}.

Figure 5.1 Leicester Points and Roads Emission Inventory

The primary aim of validation is to evaluate the accuracy of modelled data for the purpose of practical air quality management. It is worth noting that the data available for use in this project is the minimum required by the ADMS_Urban model to run dispersion calculations (Details of emission input data can be found in Chapter 4, section 4.4).

5.2.3 Meteorological Data from the Elmdon Station

The most important requirement when running air quality dispersion models, other than good emissions information, is the availability of high quality meteorological data. It is well known that weather conditions significantly affect the dispersion of pollutants (Bower, 1996). The most significant meteorological parameters that affect atmospheric dispersion are the wind direction and wind speed, the amount of vertical mixing in the air and the air temperature.

Dispersion models also need to have data available not only for the state of these variables at the surface, but also at various heights up to a level when the effects of the influence of the ground on the wind and turbulence are reduced to zero, i.e. the top of the boundary layer (Carruthers, 1992). Ideally, in order to represent the state of the atmosphere properly, a mast standing several hundred metres above ground level would need to be erected with automatic sensors placed at various levels. Clearly though this would be very expensive and difficult to set up, instead the automatic sensors are normally placed at set levels.

The meteorological data used in this project were acquired from the UK Meteorological Office. This data comprised hourly sequential values measured at the Birmingham Elmdon meteorological station (the nearest to Leicester). The data available covered the period from the 1994 to the October 1997 inclusive. The following variables were provided:

- Julian day number (TDAY),
- Local time (hours, THOUR),

- Near surface temperature (T0C (degrees)),
- Wind speed (U),
- Wind direction (angle wind is coming from in degrees clockwise from north (PHI)
- Precipitation rate (mm/hour) (P),
- Cloud cover (oktas) (CL).

The meteorological data is used by the ADMS_Urban model to calculate the boundary layer scaling parameters, i.e. boundary layer height and the reciprocal of the Monin-Obukhov length. As noted in Chapter 3, the latter is a stability parameter that new generation atmospheric dispersion models use in preference to the Pasquill-Gifford stability categories which are typically used by first generation models (Carruthers, et al. 1992).

5.2.4 Meteorological Data at Leicester

The Elmdon station was closed down at the end of 1997. However in the same year the Leicester Meteorological Mast was established and this now acts as a source of local weather data. The Leicester Meteorological Mast has provided local meteorological data since January 1997. The parameters monitored at the Leicester Meteorological Mast include;

- Dry-bulb Temperature at 2m and 10m above ground level,
- Wind direction at 10m,
- Wind speed at 10m,
- Standard deviation of the horizontal wind direction (derived),
- Standard deviation of the vertical wind speed (derived).

However the data does not include parameters such as cloud cover and heat flux which are needed by the ADMS_Urban model. It is not possible to calculate cloud cover from these parameters monitored at Leicester Meteorological Mast. However, surface heat

flux can be derived from the air temperature difference and wind speed. A detailed discussion of the use of local meteorological data in ADMS_Urban can be found in section 5.6.

5.2.4 Methodology for Validation

In practice, one of the most important roles of dispersion models in local air quality management is to be able to predict the number of exceendences of a given air quality standard for the year. The accuracy of instantaneous values is of marginal significance for air quality management. Accordingly, the principal test used here is a comparison of the measured and modelled pollutant levels based on percentiles, though it should bear in mind that monitored data is also subject to some uncertainties. A number of comparisons based on instantaneous values (i.e. time-series plots) are also made. However, the following should be noted;

- The comparison of hourly values (e.g. by correlation) is problematic because there is considerable variation in model input parameters at this time scale. A time offset between measured and modelled parameters of just 1 hour can significantly degrade what might otherwise have been a good correlation.
- Local short-term random turbulence resulting from nearby buildings cannot be accounted for by the model. This is another reason not to place too much significance on the comparison of hourly values.

In contrast to Eulerian models, which predict a volume-averaged pollution value for a relatively large box (say 100m x 100m), Gaussian plume models give a result that can be

very sensitive to the receptor location. It is a fundamental property of Gaussian plume models that there can be large pollution gradients over relatively small spatial scales. For this reason, it is important to carry out scenarios by using the either grid or receptors around AUN site and other monitoring sites. This can examine the sensitivity of the model performance according to the variation of receptor locations. A series of PV-WAVE programs were developed to carry out these comparisons (also noted in Chapter 4).

5.3 MODELLING NO_2 AND NO_X

NO_2 and NO_x modelled values are accessed in this section. Annual simulations for the period 1994 to 1997 were carried out first to gain an overall performance of the ADMS_Urban model. This was followed by consideration of monthly simulation results for selected periods. Short period time series comparison between modelled values and AUN monitored values are also analysed.

5.3.1 ADMS_Urban Annual Predictions

Nitrogen Dioxide (NO_2)

The percentile plots (see Figure5.2) indicate that ADMS_Urban predicted levels of NO_2 are generally very closed to the levels measured at the monitoring station for each year. ADMS_Urban performed well at predicting lower percentile values (about 20^{th} percentile), although it slightly over-predicted at higher percentiles, and under-predicted at lower percentiles. The average concentrations for each period are shown in Table 5.2.

Calculations of the percentage of under/over prediction throughout this chapter are based on the formula: $\frac{100*(AverageADMS - AverageAUN)}{100*AverageAUN}$.

Table 5.2 NO_2 : ADMS_Urban Annual Prediction and AUN Data Average Comparison

Year	AUN Annual Average (ppb)	ADMS Annual Average (ppb)	Percentage of under/over prediction	Correlation coefficient
1994	22.6	22.8	1%	0.58
1995	24.7	23.3	-6%	0.53
1996	22.2	24.5	10%	0.51
1997	21.3	16.5	-23%	0.65

It can be seen that correlation coefficient is not obviously related to relative difference (percentage of under/over prediction). The relative differences were of the order of -23% (1997) to just 1% for 1994 output. This variation is most probably due to varying meteorological conditions. Though it should also be noted that the emission inventory was constructed for 1996 and it has not been possible to produce a separate emission inventory for each year.

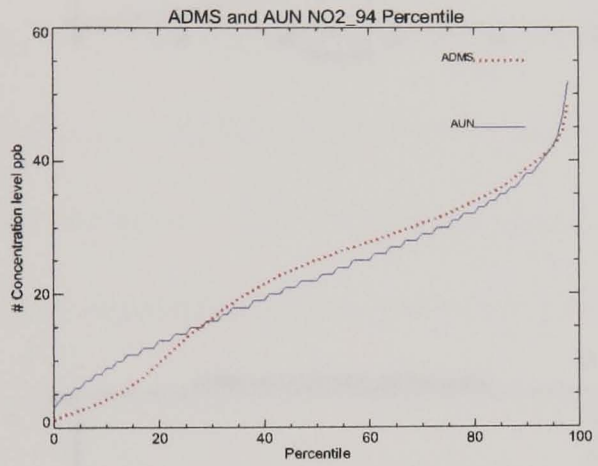
Nitrogen Oxides (NO_x)

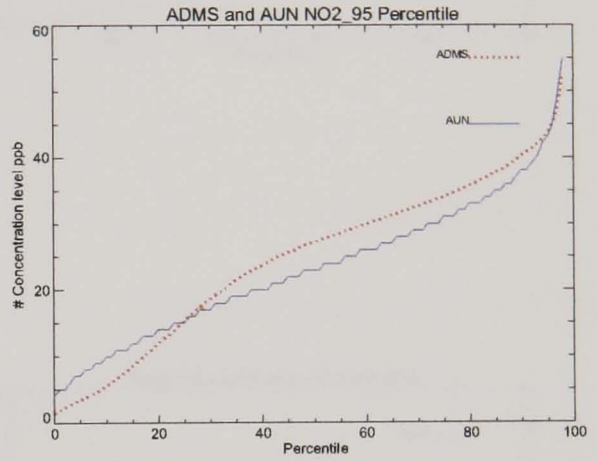
The percentile plots (Figure 5.3) clearly show that ADMS_Urban predicted levels of NO_x were generally higher than the levels measured at the monitoring station for each year. It appears that ADMS_Urban predicted values are closer to the AUN measured values at lower percentiles. The average concentrations for each period are shown in Table 5.3

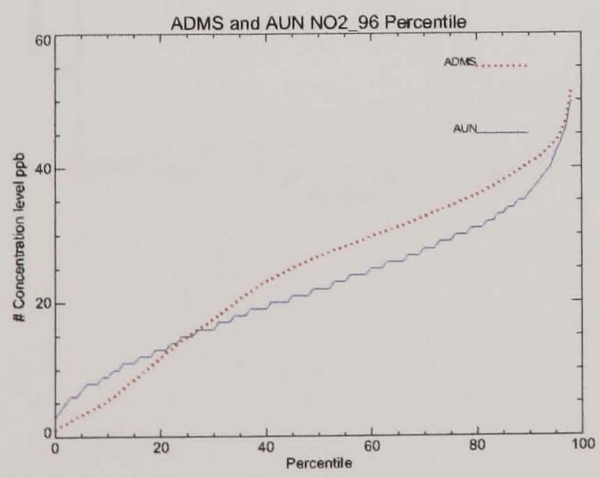
Table 5.3 NO_x: ADMS_Urban Annual Prediction and AUN Data Average Comparison

Year	AUN Annual Average (ppb)	ADMS Annual Average (ppb)	Percentage of under/over prediction	Correlation coefficient
1994	43.8	60.2	37%	0.53
1995	44.3	70.4	59%	0.45
1996	41.8	70.0	67%	0.49
1997	41.0	68.4	67%	0.46

Figure 5.2 NO_2: ADMS_Urban Annual Output and AUN Data Percentile Comparison 1994 - 1997







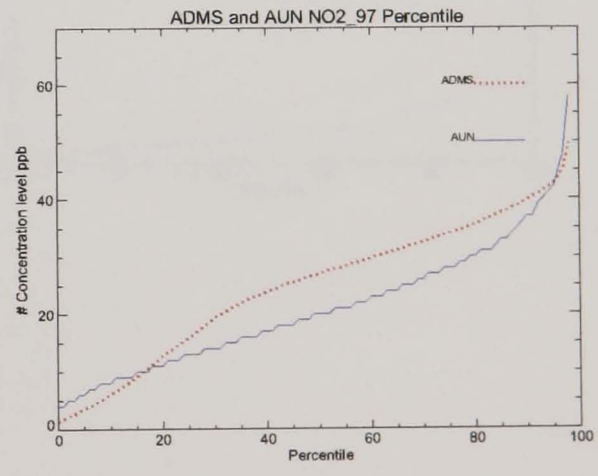
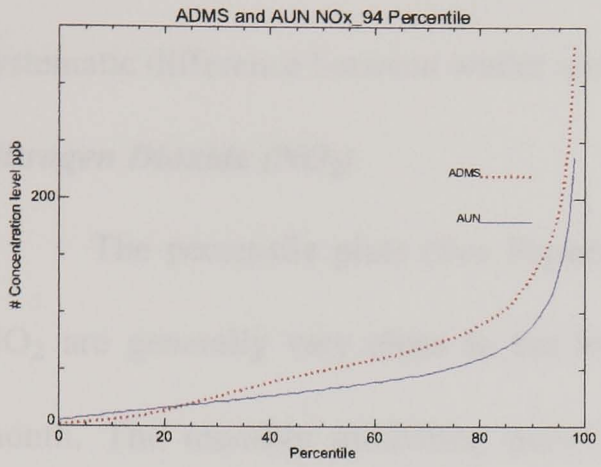
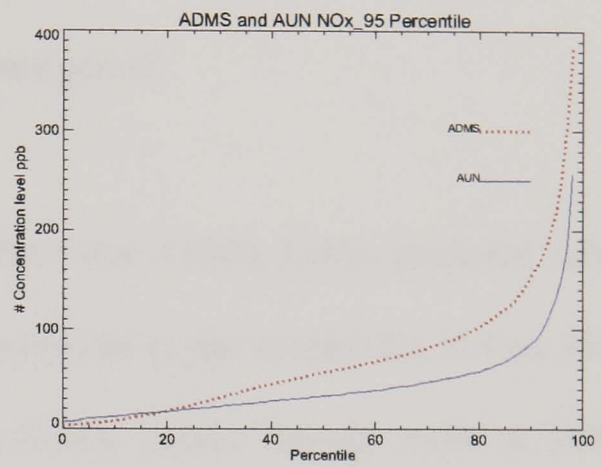
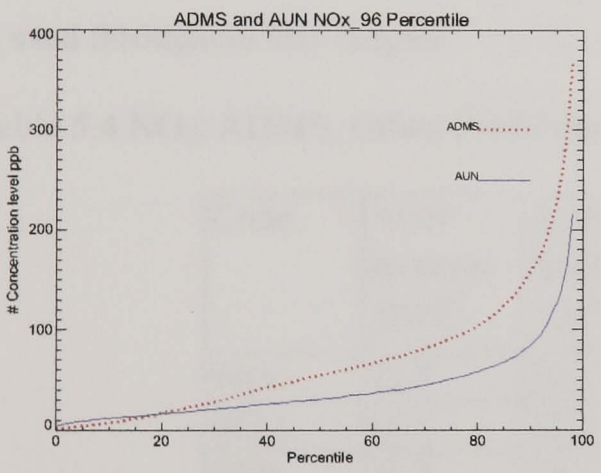
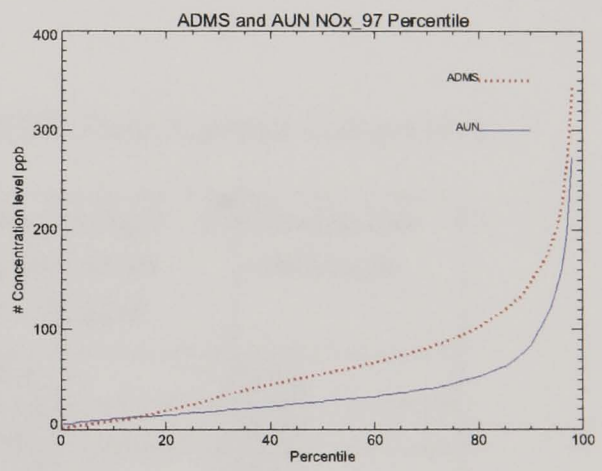


Figure 5.3 NOx: ADMS Annual Output and AUN Data Percentile Comparison
1994 - 1997









5.3.2 ADMS_Urban Monthly Prediction

Annual simulations can be seen to give generally good agreement between modelled vales and monitored values. In this section monthly comparisons are made to reveal whether the accuracy for individual month is same as for a year and whether there is a systematic difference between winter and summer period.

Nitrogen Dioxide (NO_2)

The percentile plots (See Figure5.4) show that ADMS_Urban predicted values of NO_2 are generally very close to the levels measured at the monitoring station for each month. The monthly modelling period is randomly chosen through 1994 to 1997 but includes both the summer and winter months. The average concentrations for each period are shown in Table 5.4. Codes used in this table indicated the time period of average, i.e. 9406 means the June of 1994, 9412 means December of 1996 and the same coding system is used throughout this chapter.

Table 5.4 NO_2: ADMS_Urban Prediction and AUN Data Average Comparison

Code	AUN Average (ppb)	ADMS Average (ppb)	Percentage of under/over prediction	Correlation coefficient
9406	22.5	24.2	8%	0.53
9412	16.1	21.2	32%	0.39
9506	20.7	23.2	12%	0.46
9511	24.6	18.8	-24%	-0.23
9608	19.2	24.9	30%	0.26
9612	24.4	25.1	3%	0.43
9701	21.3	16.5	-23%	0.65

The closest match of modelled values and monitored values was in June 1994 and December 1996 (Table 5.4), ADMS_Urban over-predicted by just 8% and 3% respectively. ADMS_Urban model performed well at predicting lower percentile values, i.e. about 20th percentile, although it slightly over-predicted at higher percentiles, and under-predicted at lower percentiles. For the months considered, ADMS_Urban estimated the average concentration to within -24% to 30% of the measurement value.

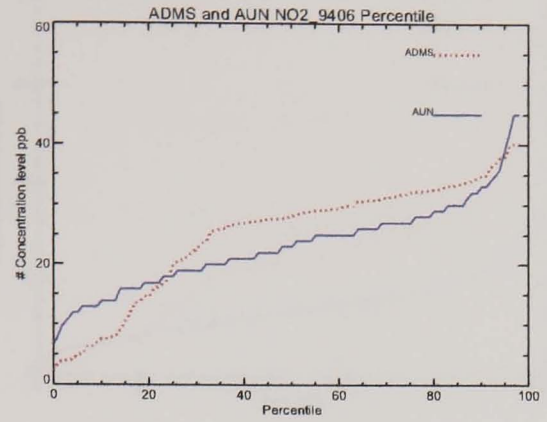
Nitrogen oxides (NO_x)

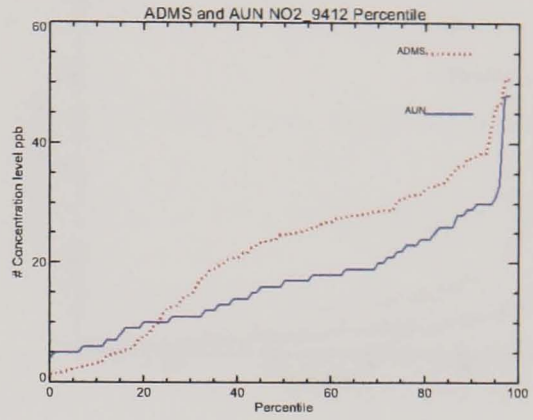
The percentile plots (see Figure 5.5) clearly show that ADMS_Urban predicted levels of NO_x are generally higher than the levels measured at the monitoring station for each month. It appears that the ADMS_Urban predicted value is closer to the AUN measured value at lower percentiles. The average concentrations for each period are shown in Table 5.5. The closest case could be found at November 1995 and January 1997, when ADMS_Urban over-predicted 14% and 15% respectively. For monthly average, the model tends to over-predict more than 50%.

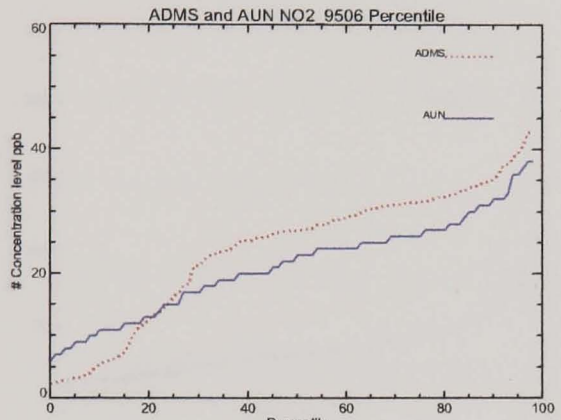
Table 5.5 NO_x : ADMS_Urban Prediction and AUN Data Average Comparison

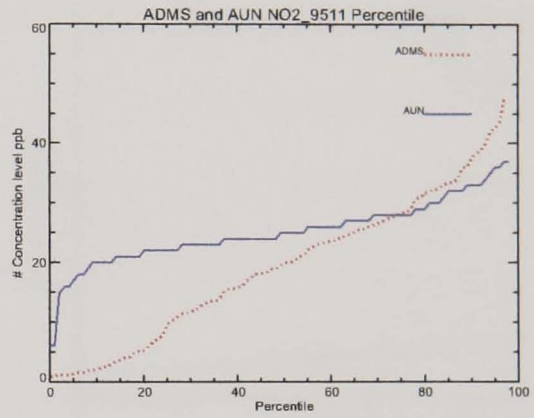
Code	AUN Average (ppb)	ADMS Average (ppb)	Percentage of under/over prediction	Correlation coefficient
9406	33.8	55.6	64%	0.5
9412	24.4	53.1	118%	0.13
9506	32.9	54.0	64%	0.31
9511	39.4	45.0	14%	0.11
9608	31.3	66.7	113%	0.17
9612	38.5	77.9	102%	0.33
9701	37.3	42.8	15%	0.73

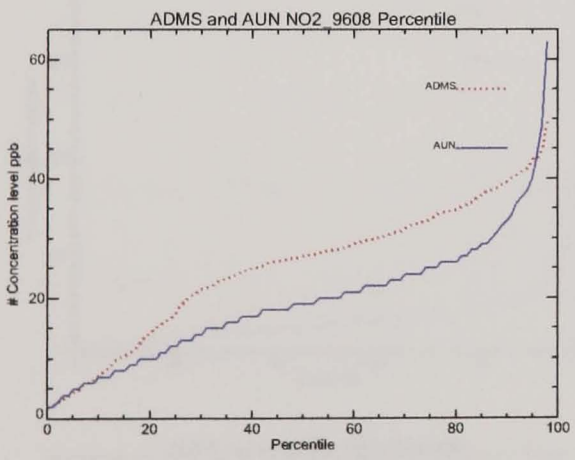
Figure 5.4 NO_2: ADMS_Urban Output and AUN Data Percentile Analysis (Monthly)

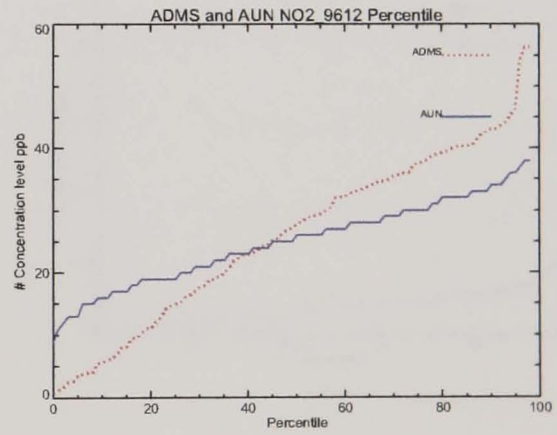












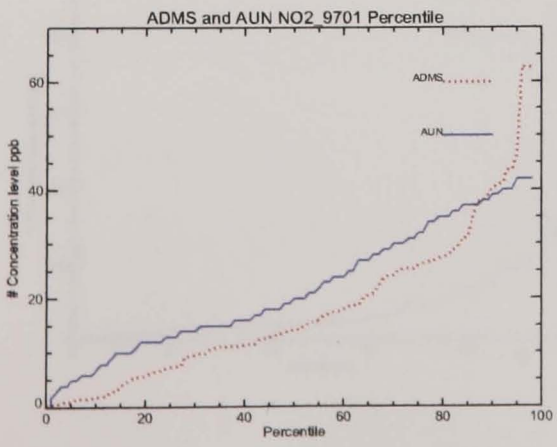
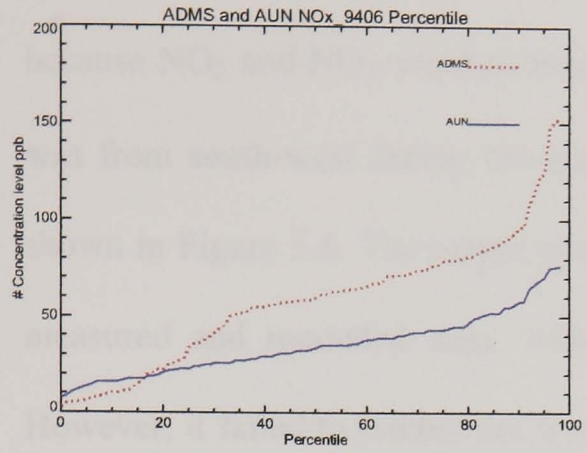
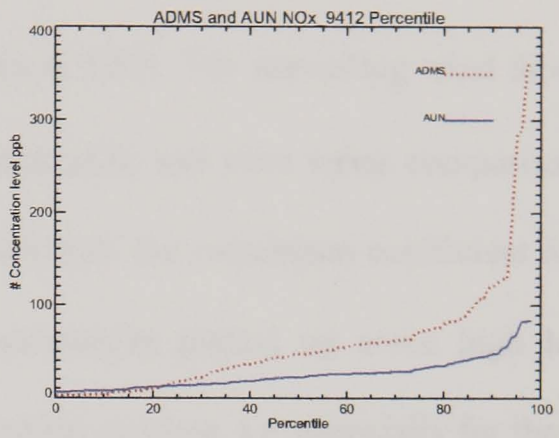
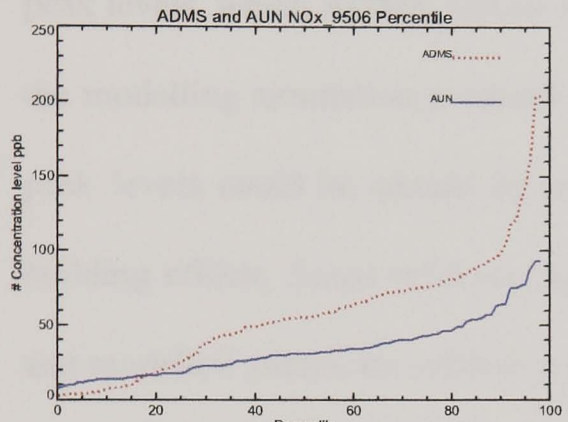
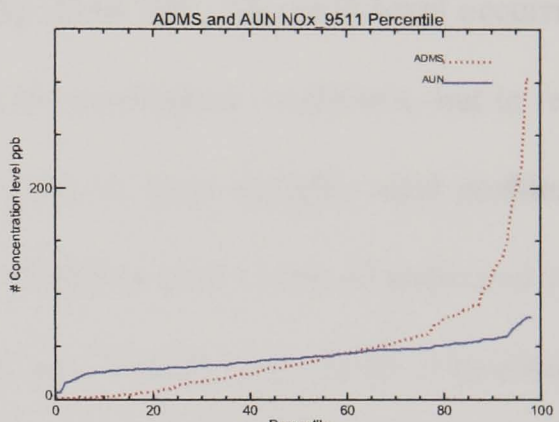


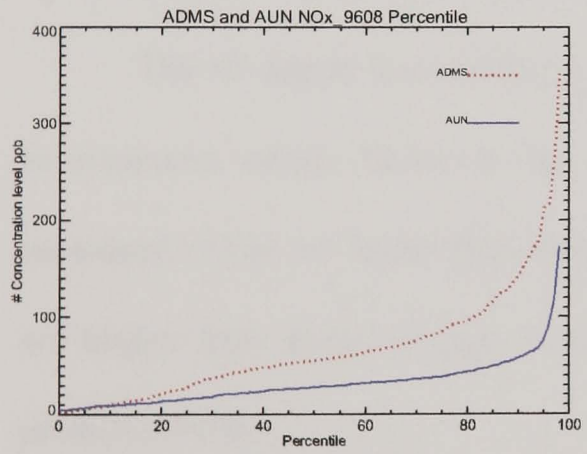
Figure 5.5 NOx : ADMS Output and AUN Data Percentile Analysis (Monthly)

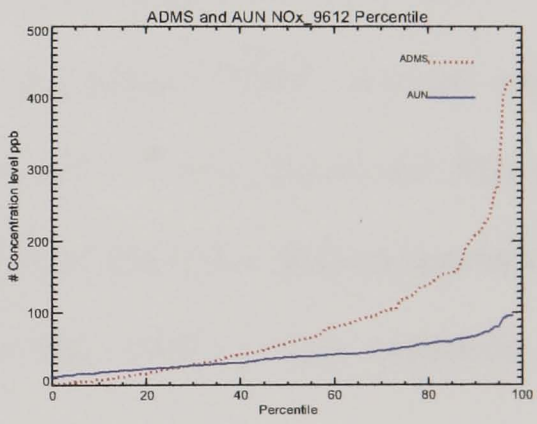


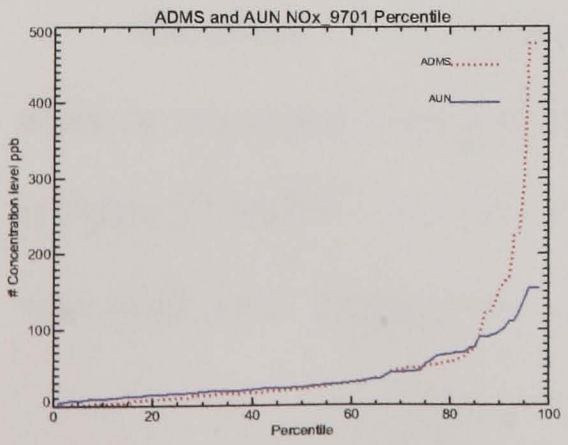












5.3.3 Pollution Incident Periods and Typical Periods Prediction

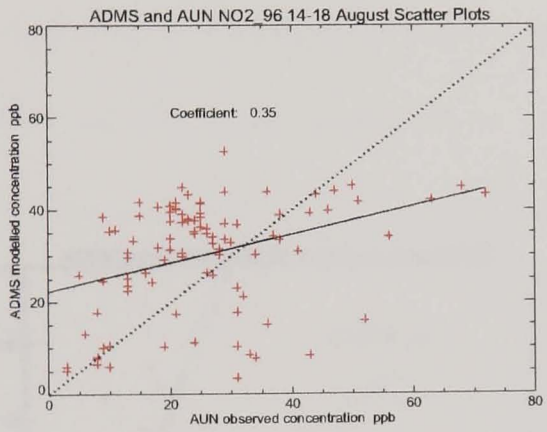
The period 14th to 18th August 1996 was chosen as a pollution incident period because NO_2 and NO_X reached their highest levels in 1996. The prevailing wind direction was from south-west during this period. The scatter plots and time series comparison are shown in Figure 5.6. The scatter plots are annotated with the correlation coefficient for the measured and modelled data. ADMS_Urban successfully picked up some high levels. However, it failed to predict the peak level or pollution incident, i.e. especially for the NO_X peak levels, which ADMS_Urban over-predicted by about 30%. The peak level occurring in the modelling simulation is mainly dependent on meteorological conditions, but in reality, peak levels could be caused by various factors, such as local specific wind profiles and building effects. Some evidence suggests that the morning peak levels of measured values and modelled values are related to the traffic rush hour, though more likely to be related to meteorological conditions because the pollution emissions for each day is the same.

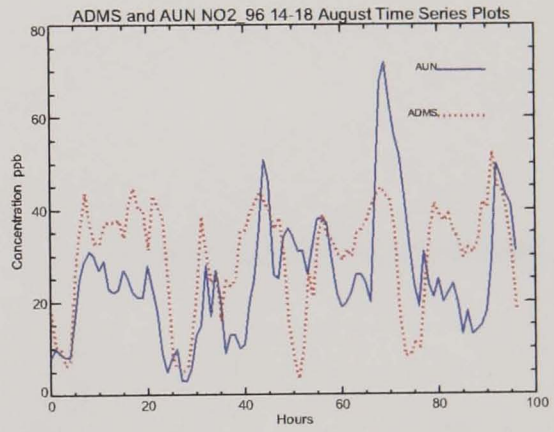
The 45 degree lines in the scatter plots indicate where modelled values are identical to measured values. However, the regression lines show over-prediction for NO_2 when measured values are lower than about 35 ppb, but under-prediction when measured values are higher than about 35 ppb. It also can be seen that ADMS _Urban constantly over-predicted NOx.

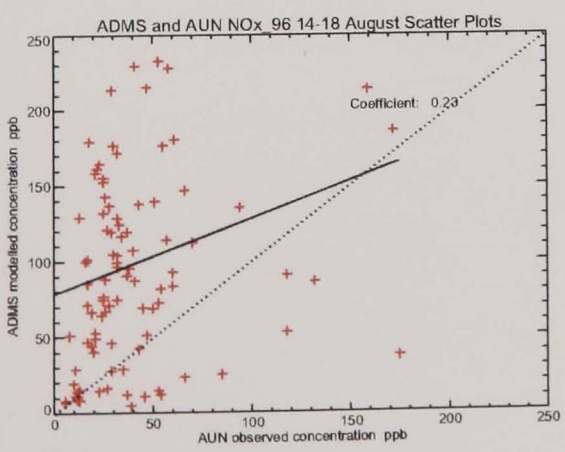
The period 1st to 5th February 1996 was chosen as a typical pollution period in which no exceedences were found. The scatter plots and time series comparison are shown in Figure 5.7. For NO_2, predicted values were lower than monitored values when the values were under about 28ppb. However, when values were over 28ppb, ADMS_Urban over-

predicted NO_2, though the predicted values and monitored values were still reasonably close. Some traffic patterns can be found in the time series plots, modelled data showed more obvious peak levels in traffic rush hours. ADMS_Urban over-predicted NOx values during this period 1. Some peak levels of modelled values and monitored values happened at similar time, but modelled values were greatly higher than monitored values. Overall, the modelled values and monitored values have good agreement for NO_2. However, the ADMS_Urban model over-predicted NO_x in most cases.

Figure 5.6 Analysis of NO_2 and NOx Pollution Incident Period 14-18 August 1996







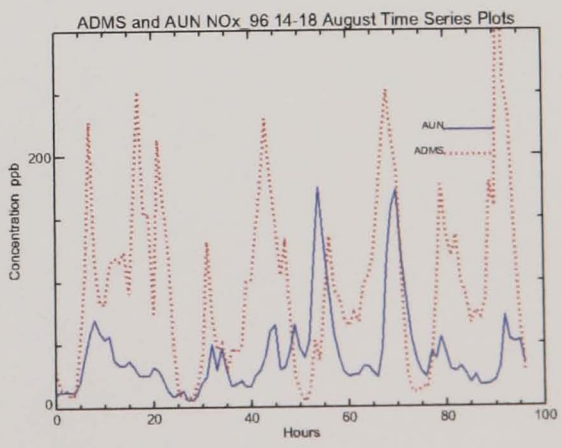
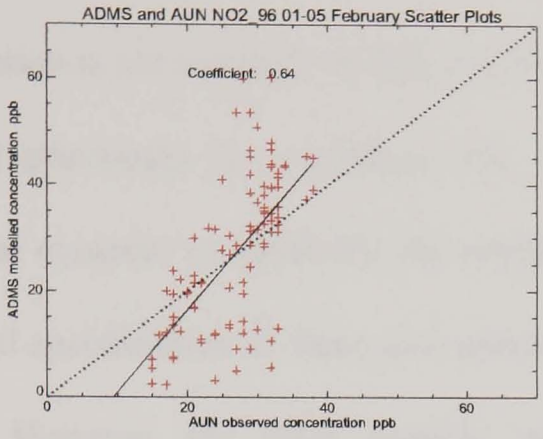
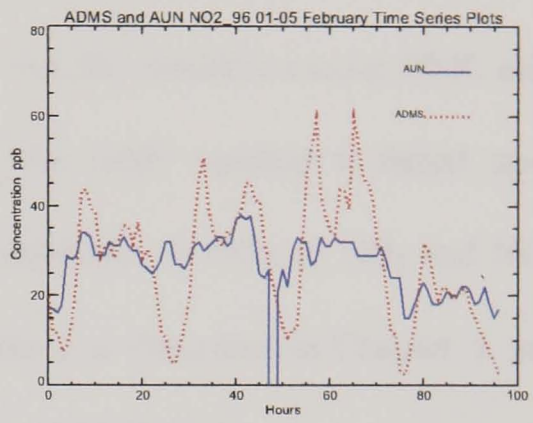
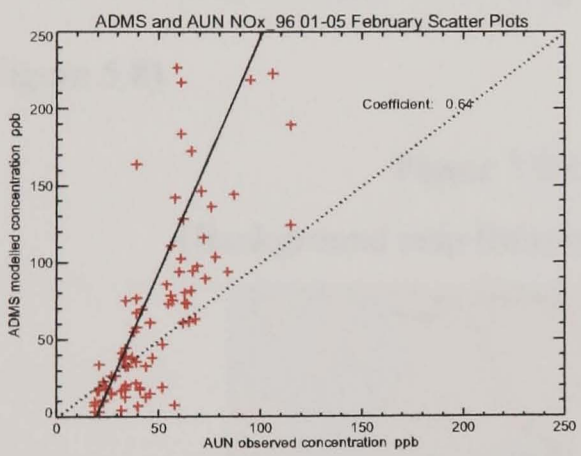
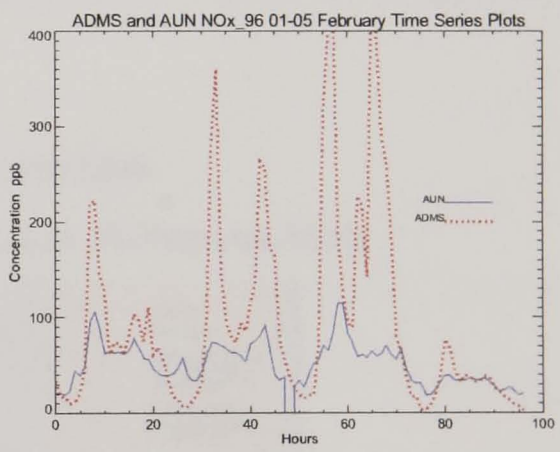


Figure 5.7 Analysis of NO_2 and NOx Typical Pollution Period









5.3.4 ADMS_Urban Chemistry Modules

There are two chemistry modules available with in ADMS_Urban, one is the Derwent-Middleton Correlation (DMC), another is the Generic Reaction Set (GRS). If the GRS option is not selected, ADMS_Urban will carry out the simulation using DMC scheme, as used previously for modelling NO_2 and NO_x. The DMC method is based upon an empirical equation to subdivide the calculated concentrations of NOx to NO_2 and NO (the technical specification of these two chemistry modules was described in Chapter 3, section 3.4.3). However the GRS module integrated in ADMS_Urban is a semi-empirical photochemical model to simulate a series of chemical reactions involving NO_2, NO, O_3 and other hydrocarbons. The Generic Reaction Set (GRS) requires the rural background data for NO_2, NO and O_3 (and hydrocarbons if available). Therefore, according to the wind directions, following six rural stations around Leicester were selected as background sites (see Figure 5.8).

Figure 5.8 O_3 Background Sites

(Background map from http://www.le.ac.uk/maps/uk.html)

Note in this figure -

1. Ladybower 310 - 360 degrees
2. Bottesford 0 - 70 degrees
3. Wicken Fen 70 - 140 degrees (only available for 1998)
4. Sibton 70 - 140 degrees (for 1995, 1996 and 1997)
5. Harwell 140 - 230 degrees
6. Aston Hill 230 - 310 degrees

Predictions for O_3 are only available if the GRS scheme has been used. Only O_3 values, or NOx, NO_2 and O_3 values all together can be taken into model calculation by including them in the background file. Imported 1997 national O_3 background level for Leicester, national remote O_3, NO_2 and NO_x background for Leicester, Leicester AUN O_3 background respectively were taken to GRS scheme. If all NO_x, NO_2 and O_3 are used in the simulation (including in the background file), the concentration will be the background values plus various influence the travel of the plume is having. For example, if under South West wind conditions, all the pollution would travel to the North East. Therefore, when plotting the O_3 concentration, the values where the plume did not land will only be the specified background. Where the plume lands, a decrease in O_3 will be likely to happen as it is consumed to produce NO_2. If NO_x and NO_2 are not included in the simulation (in the background file), then it is assumed that the only source of NO_x is from the plume which will react with the background O_3.

The effects of using the GRS method are shown in Figure 5.9, 5.10, 5.11 and Table 5.6. For 1997, the ADMS_Urban with GRS scheme show that NO_2 level is higher than that with Derwent-Middleton Correlation scheme. As NO_2, NOx and O_3 background values

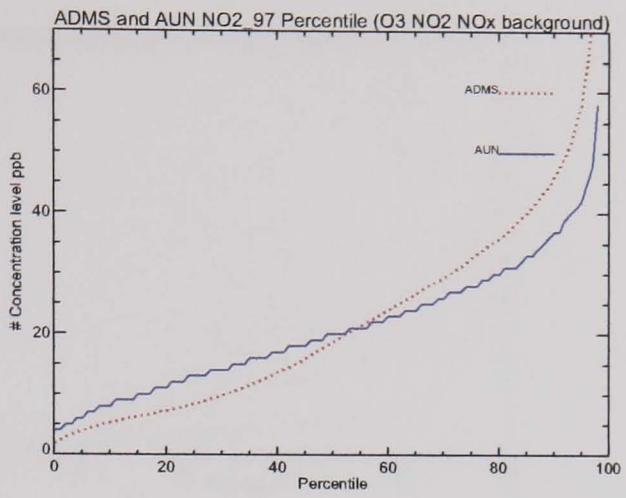
were taken into simulation, the most effective chemistry reactions were those involved NO_2, NOx and O_3, i. e. $NO_2 + h\nu \rightarrow NO + O_3$ and $NO + O_3 \rightarrow NO_2$ (also see section 3.4.4 for other reactions).

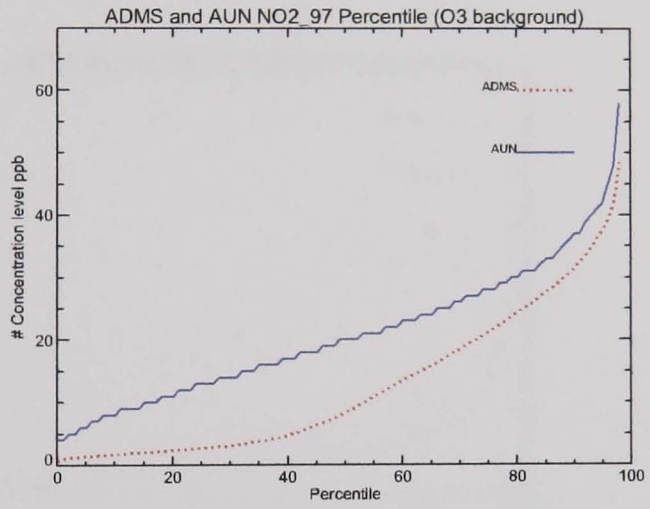
Table 5.6 ADMS_Urban Outputs with Different GRS Scheme (Meteorological Data 1997) (Annual Average)

Pollutant	Remote O_3 Background	Remote NO_2 NOx and O_3 Background	Leicester AUN O_3 Background	Without GRS Scheme	AUN Monitored
NO_2 (ppb)	12.8	22.5	8.3	16.5	21.0
NOx (ppb)	68.4	79.8	68.4	68.4	41.0
O_3 (ppb)	18.2	18.3	12.8	n/a	18.9

The results were summarised in Table 5.6. Comparing with the simulation without GRS scheme, NO_2 modelled values were higher as more O_3 converted to NO_2 when remote NO_2 , NO_x and O_3 values were taken into simulation. If only O_3 values being taken into simulation, NO_x modelled levels maintained same because there were no NOx background involved in the simulation. The percentile comparison between modelled NO_2, NOx and O_3 and measured NO_2, NO_x and O_3 can be found in Figure 5.9, Figure 5.10 and Figure 5.11. Using the GRS scheme by including remote O_3, NO_2 and NO_x background values, the ADMS_Urban model gives better prediction of NO_2 and NOx than that without background values.

Figure 5.9 GRS Scheme: NO_2 Output Percentile Analysis





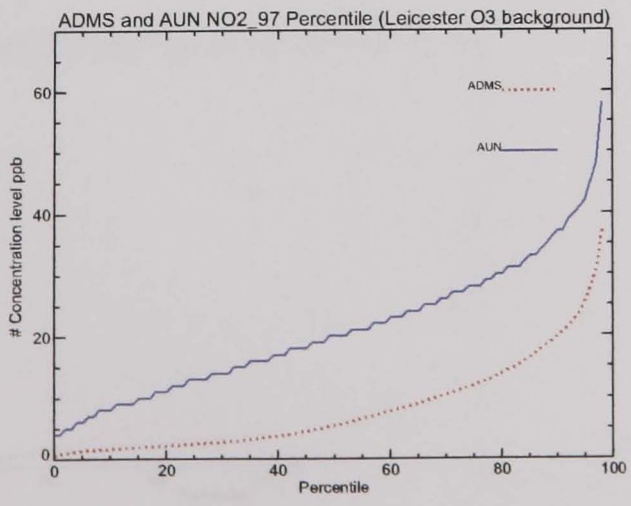
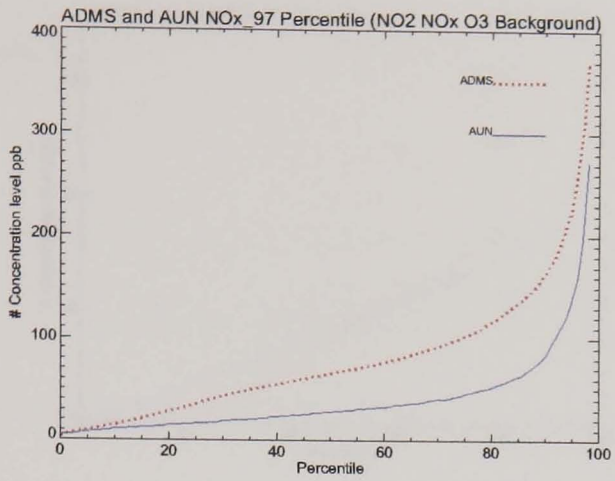
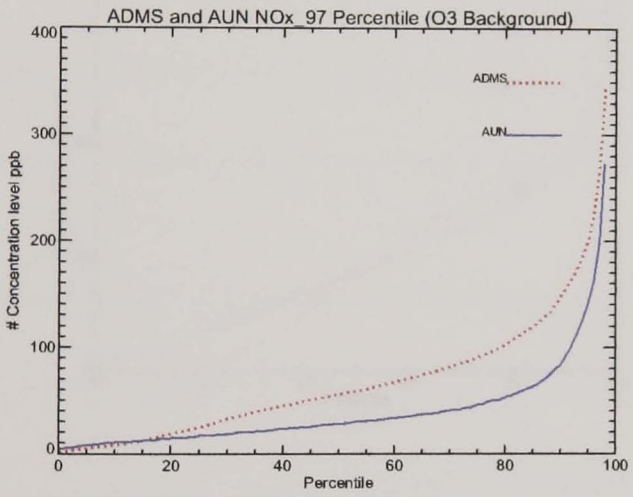


Figure 5.10 GRS Scheme: NO_x Output Percentile Analysis





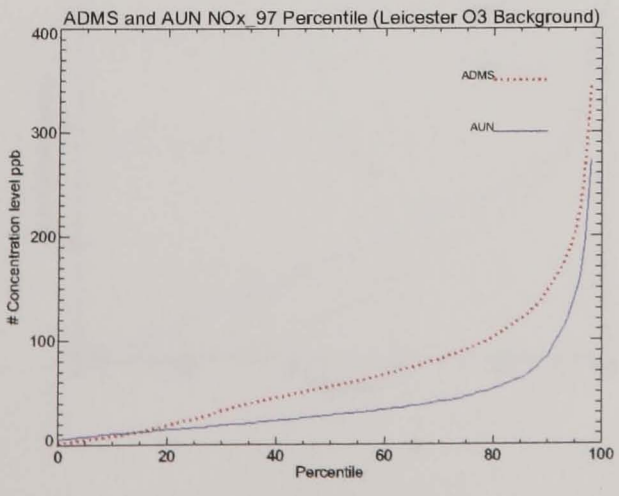
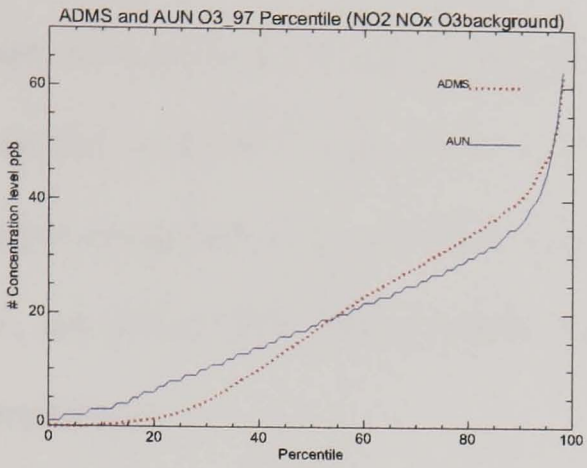
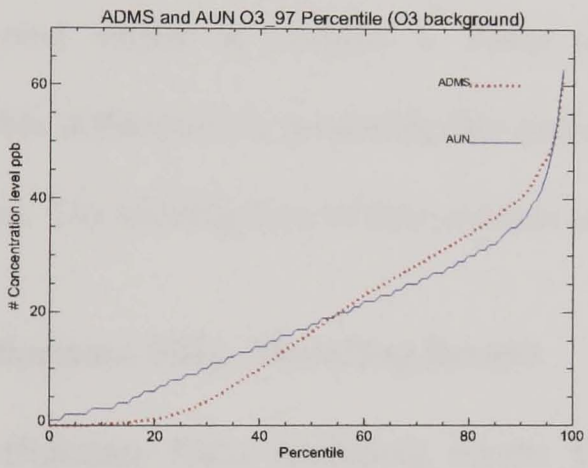
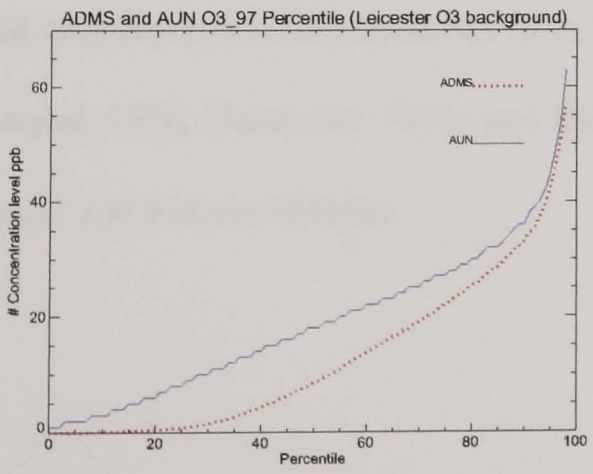


Figure 5.11 GRS Scheme: O_3 Output Percentile Analysis







5.3.5 Summary

Comparisons of modelled NO_2 and NOx with AUN measurements were made in this section. It has been shown that ADMS_Urban annual predictions for NO_2 and NOx are better than that of monthly predictions or short-term predictions. It appears that there are large random errors, but not consistent bias, in the model predictions. When modelling NO_2 and NOx, use of the GRS scheme where background data is available will improve the needed predictions.

5.4 MODELLING PM_{10}

As noted earlier in chapter 1, PM_{10} comes from various sources, this causes considerable difficulties in modelling this pollutant. PM_{10} modelled values are assessed in this section. The investigation of this complex situation is carried out.

5.4.1 Preliminary PM_{10} Modelling Results

Preliminary PM_{10} modelling results for annual and monthly simulations were obtained. The comparison of modelled value and monitored values used the same procedure for PM_{10} as for NO_2 and NOx in previous section. Annual predictions were for year 1994-1997, and monthly predictions included June 1994, December 1994, June 1995, November 1995, August 1996, December 1996, and January 1997, which were chosen randomly to cover winter and summer months.

PM_{10} Annual Predictions

The percentile plots (Figure 5.12) clearly show that ADMS_Urban predicted levels of PM_{10} are consistently significantly lower than the levels measured at the AUN station. The average concentrations for each period are shown in Table 5.7.

Table 5.7 PM_{10}: ADMS_Urban output and AUN data Average comparison ($\mu g/m^3$)

Year	AUN Annual Average ($\mu g/m^3$)	ADMS Annual Average ($\mu g/m^3$)	Percentage of under/over prediction	Correlation coefficient
1994	21.5	6.08	-72%	0.38
1995	20.1	7.11	-65%	0.34
1996	21.6	7.21	-67%	0.24
1997	20.9	7.14	-66%	0.36

The evidence from annual percentile comparisons suggests a shortfall for modelled levels throughout 1994 to 1997. The difference between modelled values and AUN monitored values were greater in the high percentiles, e.g. over 60^{th} percentile, but slightly smaller at low percentile, e.g. below 20^{th} percentile.

Monthly PM_{10} predictions

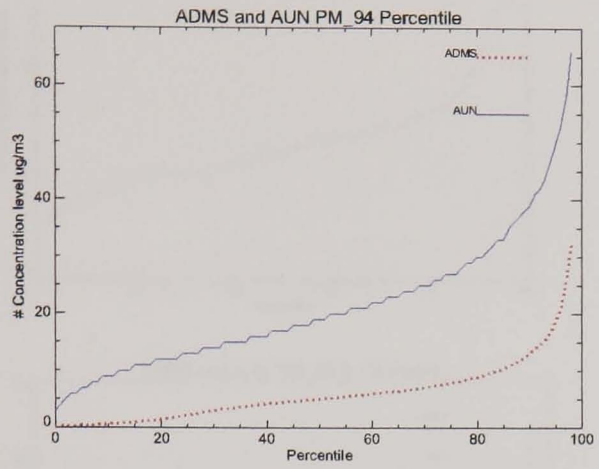
The percentile plots clearly show that ADMS_Urban predicted levels of PM_{10} are also constantly lower than the levels measured at the AUN station (Figure 5.13). The average concentrations for each period are shown in Table 5.8. The under-prediction of PM_{10} in ADMS_Urban could be up to 70-80% (Table 5.8).

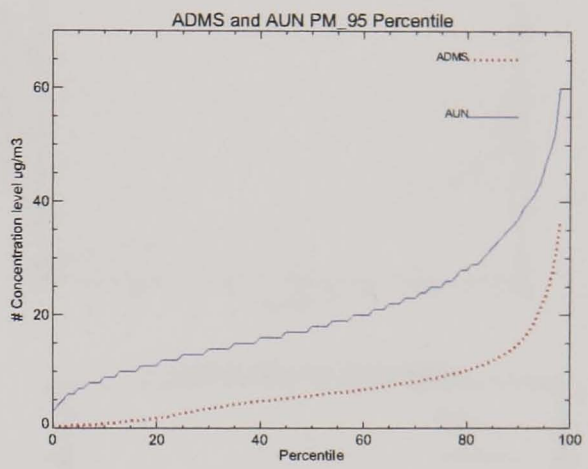
Table 5.8 PM_{10} : ADMS_Urban output and AUN data Average comparison

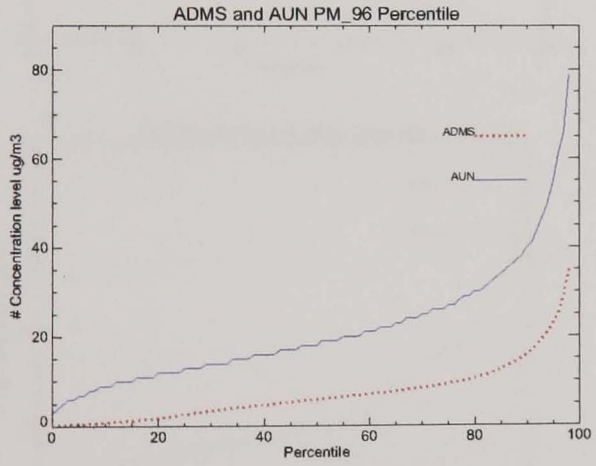
Code	AUN Average ($\mu g/m^3$)	ADMS Average ($\mu g/m^3$)	Percentage of under/over prediction	Correlation coefficient
9406	25.3	5.11	-80%	0.63
9412	8.3	5.09	-39%	-0.2
9506	17.9	5.41	-70%	0.2
9511	17.2	5.66	-67%	-0.34
9608	21.6	6.58	-70%	0.14
9612	15.4	8.14	-47%	-0.1
9701	19.1	5.38	-72%	0.41

Overall, ADMS_Urban under-predicted PM_{10} levels across the years, however, occasionally, e.g. December 1994 and December 1996, ADMS_Urban over-predicted at high percentiles, i.e. at 90-95th percentile. It appears that the variations of ADMS_Urban monthly predictions are greater than that of annual predictions. This pattern is also reflected on the predictions for NO_2 and NOx as noted earlier. Modelled results suggest that it does not explain the levels observed. This leads to the further examination of the reason of this under-prediction.

Figure 5.12 PM_{10}: ADMS_Urban Annual Output and AUN Data Percentile Comparison 1994 -1997







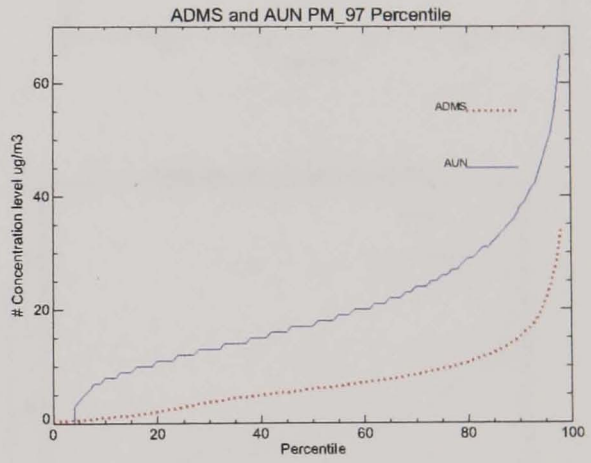
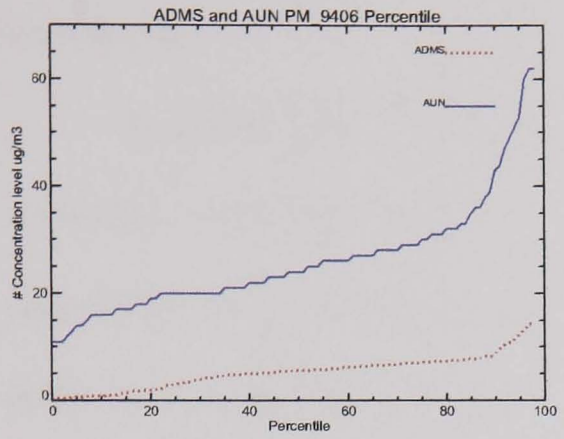
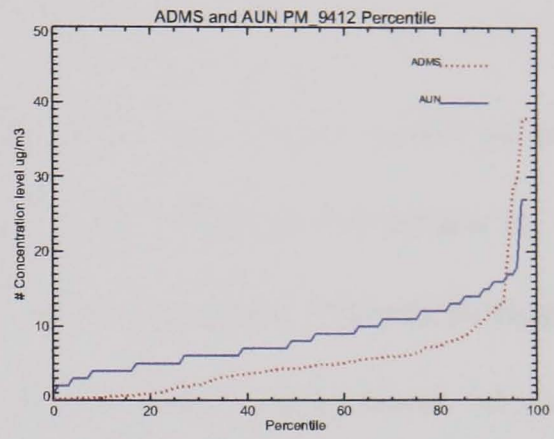
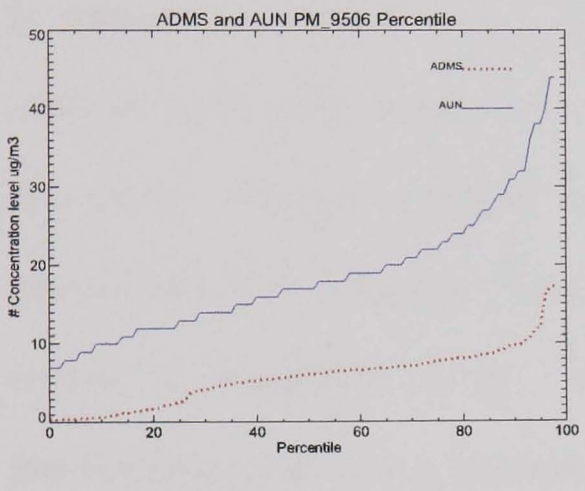
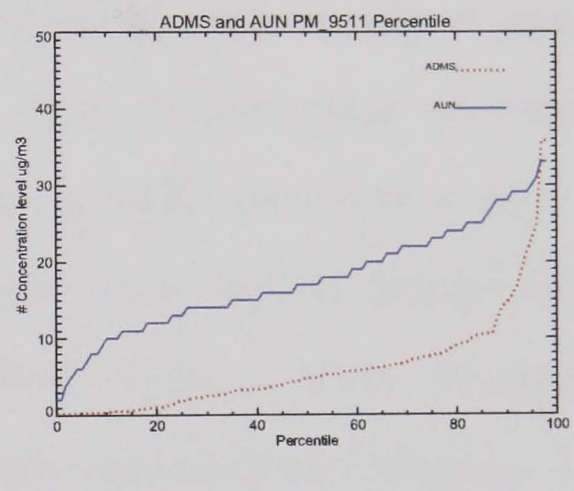


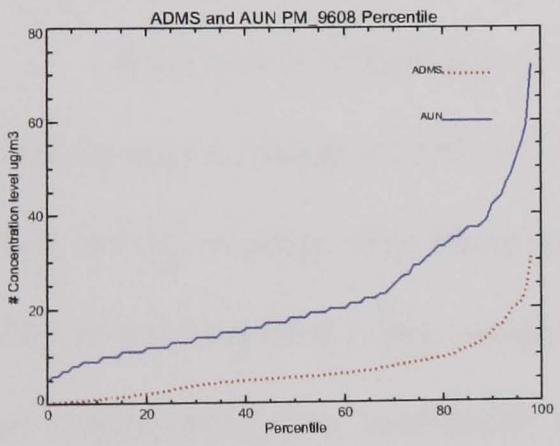
Figure 5.13 PM_{10}: ADMS_Urban Output and AUN Data Percentile Analysis (Monthly)

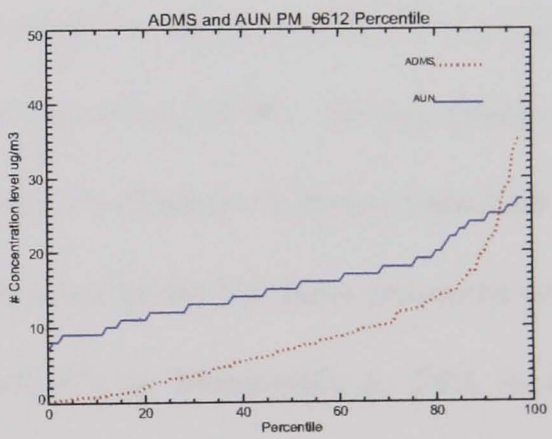


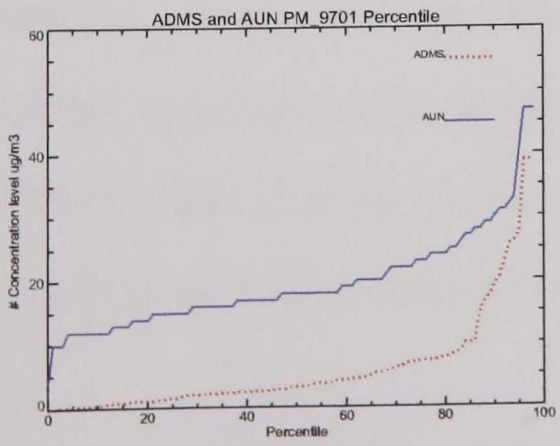












5.4.2 Sources of PM_{10} Particulates Matters

In order to find the reason for PM_{10} under-prediction, the nature of PM_{10} need to be considered.

In general, PM_{10} is derived from a wide range of sources: it can be primary or secondary, man-made or natural in origin. Recent investigations (Harrison et. al, 1997) suggest that PM_{10} can be roughly divided into three categories. Primary particulates to a large extent comprise those derived from incomplete combustion in motor vehicle engines or stationary combustion plant. Secondary particulates consist largely of ammonium sulphate, ammonium nitrate and secondary organic aerosols, which are formed by atmospheric oxidation of sulphur dioxide, nitrogen oxides and volatile organic. Such aerosols take time to form and can be transported over considerable distances, including sources in continental Europe. Coarse particles include a variety of natural and anthropogenic material, e.g. wind-blown dust and biological matter such as spores.

Road traffic related sources of PM_{10} contribute approximately 25% of the annual total emissions taking the UK as a whole (Harrison et. al, 1997). The percentage in urban area is very variable, depending on the presence or absence of major industrial sources. Recent emission inventories complied for urban areas in the UK have estimated percentage of contributions from road traffic ranging from 8% in Merseyside to 58% in the West Midlands (Huchinson and Clewley, 1996). The percentage is likely to be even higher in London. In Leicester, in the absence of major industrial sources, on would also expect a relatively high percentage. Regression analysis comparing measured PM_{10} concentrations with those of CO have indicated that traffic exhaust related sources contribute about 40-

50% of the measured winter mean PM_{10} concentrations in UK cities (Buckingham et. al, 1997). This contribution can be greater during winter episodes of elevated concentrations due to poor dispersion of local primary emissions. There can also be a contribution to primary PM_{10} for coarse particles from non-combustion related sources such as wind blown soil and dust and sea spray (QUARG, 1996).

The contribution of secondary particles to measured PM_{10} is much more uniform across the country than that of the primary particles because the secondary particles are formed relatively slowly in the atmosphere and have a long atmospheric lifetime (Stevenson et al., 1995).

Monitoring of PM_{10} levels in the UK has been largely based upon the use of Tapered Element Oscillating Microbalance (TEOM) analysers (APEG, 1999) and these are used in AUN stations. A principal concern with the TEOM instrument is that the filter is held at an elevated temperature (50°C) in order to minimise errors associated with the evaporation and condensation of water vapour. This can lead to the loss of the more volatile species (some hydrocarbons, nitrates etc) and has led to the identification of differences between TEOM and gravimetric measurements (i.e. BAM) at co-located sites. Gravimetric instruments also have the potential to lose some volatile particles, especially ammonium nitrate, the proportion of which is dependent upon the history of the sample (More detailed discussion about the PM_{10} monitoring instrument can be found in Chapter 6, section 6.3.2).

PM_{10} concentrations are monitored in the UK national air quality monitoring networks using TEOM instruments (Bower et. al, 1996). Monitoring of PM10 commenced in 1992 and by 1996 was monitored at over 20 sites.

The UK Expert Panel on Air Quality Standards has recommended an air quality standard for PM_{10} of 50 μg/m3 measured as a 24-hour running mean (EPAQS, 1995). The UK government has set an objective within the Air Quality Strategy that this standard should be achieved in the UK by 2005 at the 99^{th} percentile (DOE, 1997). That is, no more than four days should exceed this concentration for a full year's monitoring. This is generally considered to be a demanding target and estimates of whether or not it can be achieved, need to take into account the influence of the long-range transport of particles into the UK.

In the Leicester emission database, primary sources of PM_{10} can be incorporated.

5.4.3 Evidence for Imported PM_{10}

Following the above discussion, PM_{10} episodes at AUN sites and meteorological data analysis were examined to reveal whether any similarity in the patterns of PM_{10} levels at different cities.

Wind rose probability Plots

The original data sets used in this analysis were:

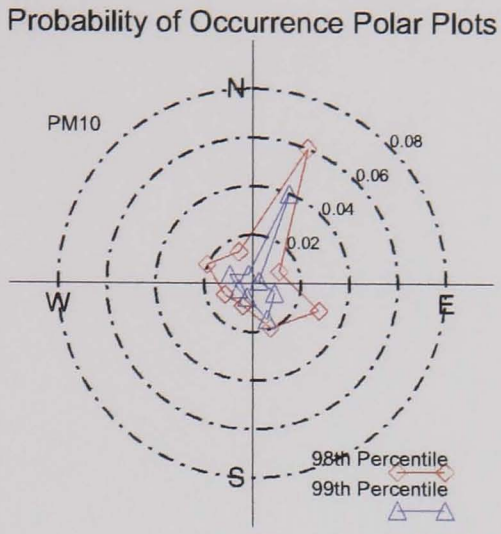
- PM_{10} data from Leicester, Birmingham and Birmingham east AUN 1994 data,
- Leicester, Birmingham and Birmingham east AUN 1995 data
- Leicester, Birmingham and Birmingham east AUN 1996 data
- 1994, 1995 and1996 meteorological data from Birmingham Elmdon station.

Birmingham, Birmingham East and Leicester AUN sites are geographically close to each other, and they have similarly historical meteorological conditions with the Elmdon station located relatively close to all three sites.

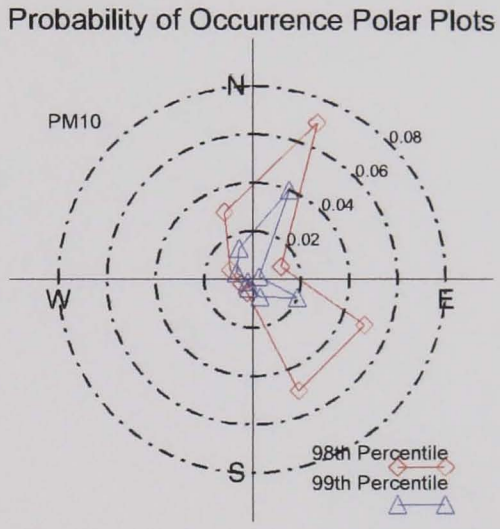
The probability of occurrence from AUN data sets shows there are similar patterns of high percentile PM_{10} value distributions through three sites each year, but for different years, the patterns are slightly changed (see Figure 5.14, Figure 5.15, Figure 5.16). Overall, PM10 peak levels almost always occurred when winds were from the North East.

Relating to the probability of high PM_{10} levels to wind directions, it can be seen that the 99^{th} percentile PM_{10} values in 1994 at Birmingham East, Birmingham and Leicester were most likely to occur (probability is over 0.06) when wind was from north-east (Figure 5.14). This situation was similar in 1995 and 1996, though the probability of 99^{th} percentile was between 0.04 to 0.06 at north-east wind direction in 1996 (Figure 5.16). This suggests that PM_{10} peak levels occurred under similar wind conditions - when winds were from North East. However, as noted earlier, the prevailing wind direction as measured at Elmdon station was from South West. These results suggest that PM_{10} peak levels were likely to occur at opposite prevailing wind directions. This is also proved next by the wind direction and wind speed plots (Figure 5.17).

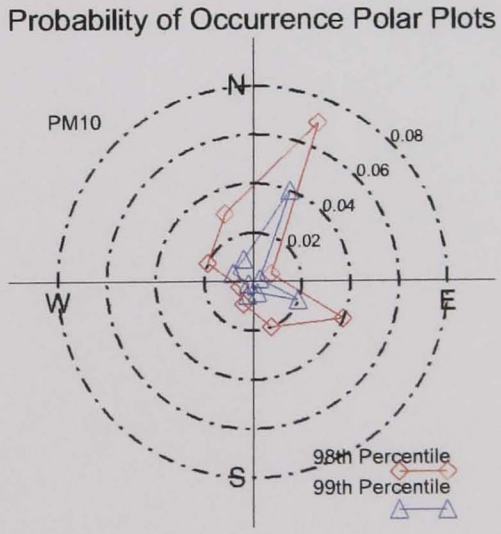
Figure 5.14



Wind Direction and AUN PM10 1994 Birmingham East

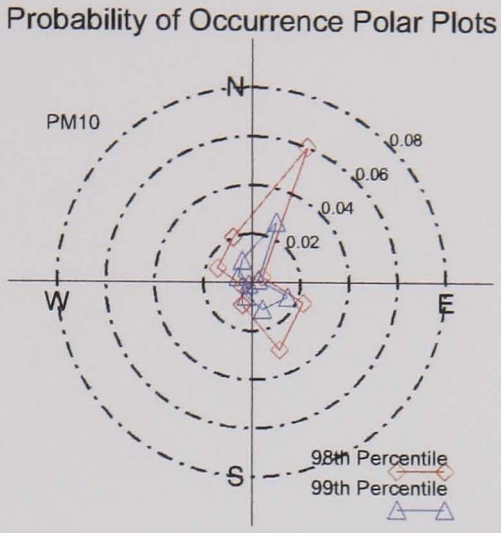


Wind Direction and AUN PM10 1994 Birmingham

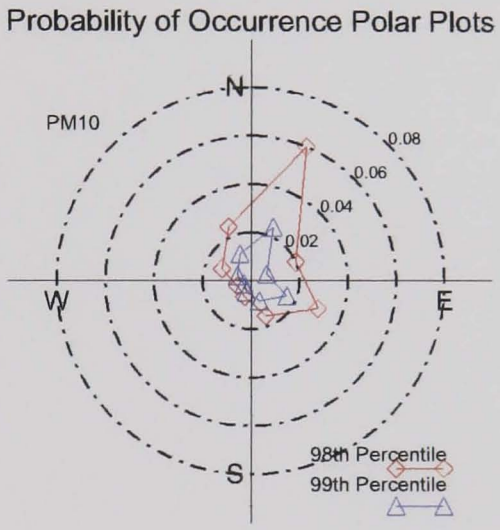


Wind Direction and AUN PM10 1994 Leicester

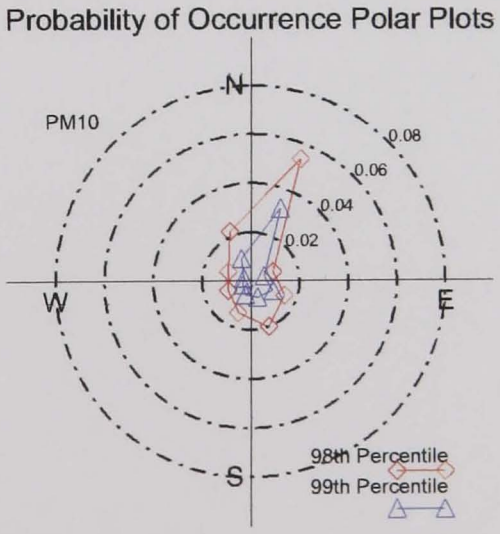
Figure 5.15



Wind Direction and AUN PM10 1995 Birmingham East

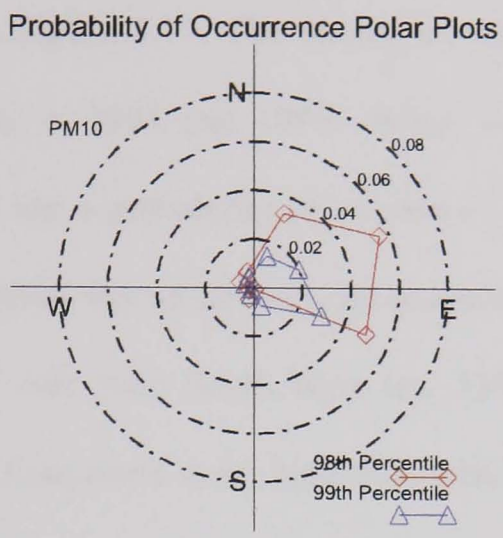


Wind Direction and AUN PM10 1995 Birmingham

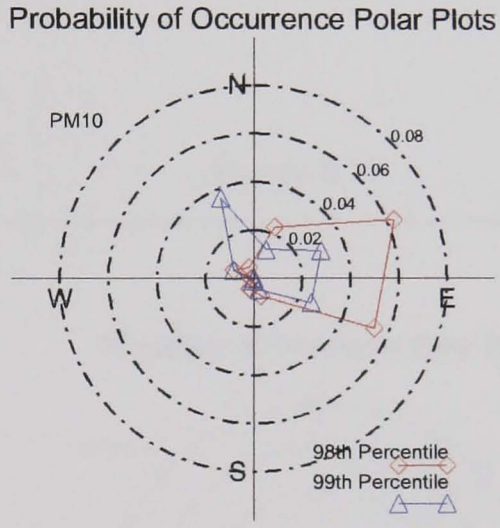


Wind Direction and AUN PM10 1995 Leicester

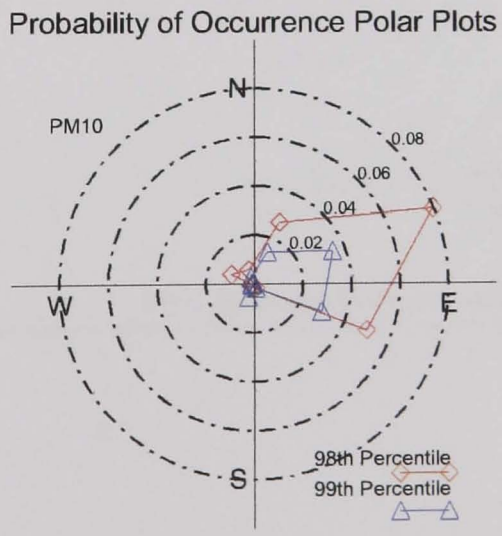
Figure 5.16



Wind Direction and AUN PM10 1996 Birmingham East



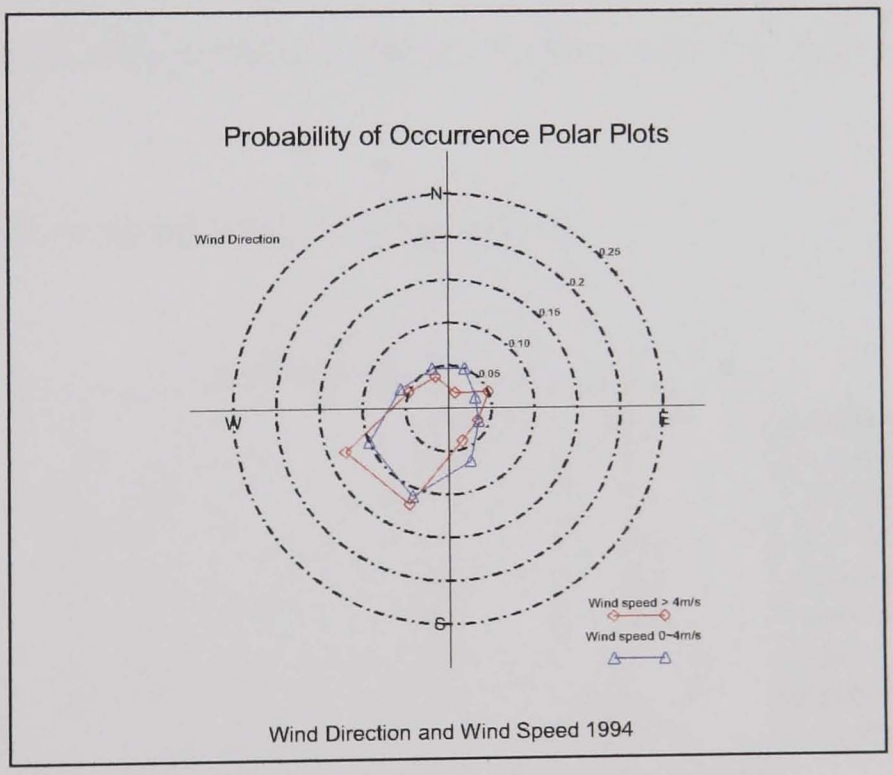
Wind Direction and AUN PM10 1996 Birmingham



Wind Direction and AUN PM10 1996 Leicester

The distribution pattern of probability of wind direction and wind speed occurrence polar plots are shown in Figure 5.17. The annual average wind speed was 4.2 m/s in Leicester in 1994 (similar in 1995 and 1996). When wind speed was over 4m/s, the prevailing wind direction has a probability of occurrence between 0.1 to 0.15 was from South West. When wind speed was under 4m/s, the prevailing wind direction as probability of occurrence around 0.1 was from South West too. This suggests the prevailing wind direction in Leicester was from south-west. However, peak levels of PM_{10} were most likely to occur when wind direction was from opposite north-east as shown previously in Figure 5.14, 5.15 and 5.16.

Figure 5.17



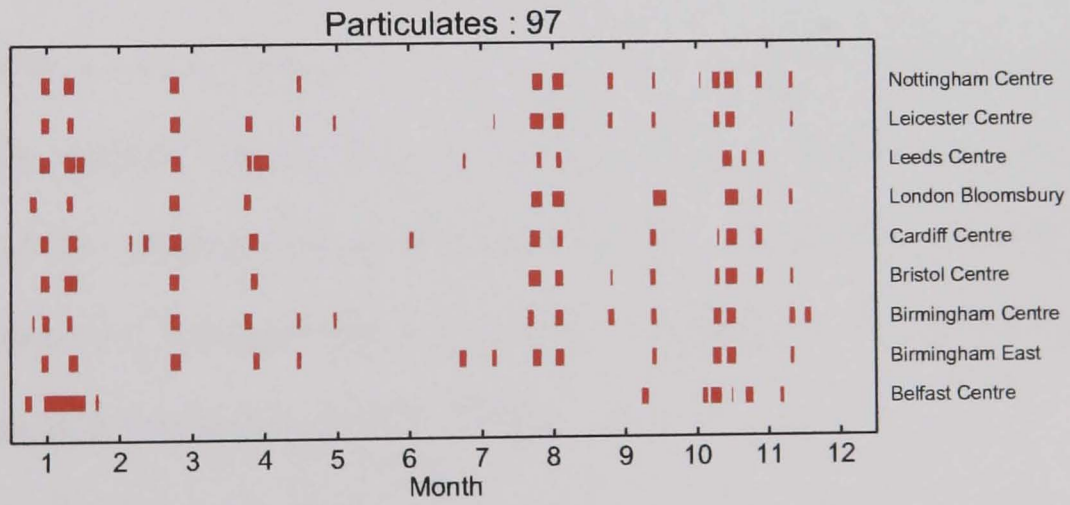
Low Pass Filtered time series plots

For the selected AUN sites, the top five percentile for each time series which has been filtered with a low pass filter are plotted in Figure 5.18. The purpose of these plots is to show the persistent features in time series, by removing the short time scale variations.

This figure shows PM_{10} peak level occurred approximately simultaneously across the country. It can be seen, in Figure 5.18, during the end of February, nearly all the AUN monitoring sites recorded values over 95^{th} percentile at the same period in the year 1997 (e.g. Nottingham centre, Leicester centre, Leeds centre, London Bloomsbury, Cardiff centre, Bristol centre, Birmingham centre, Birmingham East). Similar patterns are repeated throughout those AUN monitoring stations in the end of January, July and early August. This provides evidence that PM_{10} is a nation wide pollutant.

These analyses also provided evidence for PM_{10} imported matters as discussed earlier.

Figure 5.18 Low Pass Filtered Time Series Plots



5.4.4 Modelling Imported PM_{10}

As the previous sections have shown, apart from local primary sources, PM_{10} is also imported from non-local sources and this can have a significant impact of total PM_{10} levels. This section introduces a method to distinguish between the primary and secondary particle contributions during period of elevated PM_{10} in the UK.

Research shows that secondary particles form the main contribution to high concentrations during PM_{10} episodes. This has been demonstrated (King and Dorling 1997 and Stedman, 1997) by the comparison of urban concentrations with those in rural areas, showing that rural concentrations were similar during these episodes. In addition, the PM_{10} concentrations in urban areas during these episodes did not show the type of strong diurnal variation that would be associated with the poor dispersion of primary particles from local combustion sources. King and Dorling (1997) and Stedman (1997) also pointed out that these episodes wee characterised by winds from the east bringing long range transported secondary particles to the UK from the continent.

There is a clear relationship between the non-combustion component of PM_{10} and atmospheric sulphate concentrations (Stedman, 1997). Sulphate levels provide a good indicator of the concentration of secondary particles. A technique has been developed which enables the measured daily mean PM_{10} concentration at a monitoring site to be divided into three components (APEG, 1998):

- primary combustion particles
- secondary particles
- 'other' particles (coarse)

A regression analysis was carried out to determine the correlation coefficients *A* and *B* for primary combustion and secondary particle concentrations (Stedman, 1998), (see Table 5.9).

Table 5. 9 Regression coefficients for Black Smoke and Sulphate Receptor Modelling of 1996 PM_{10} data (Source: Stedman, 1998)

Monitoring station	Smoke coefficient, A	SO_4 coefficient, B	Intercept, C	r^2
London Bloomsbury	0.64	2.26	10.96	0.78
Birmingham Centre	0.59	2.41	8.30	0.71
Bristol Centre	1.03	2.35	10.83	0.70
Manchester Piccadilly	0.60	2.46	9.77	0.74
Newcastle Centre	0.66	3.13	7.73	0.84
Belfast Centre	0.71	2.30	9.21	0.79
Edinburgh Centre	0.59	2.46	9.85	0.61
Liverpool Centre	0.92	2.46	9.79	0.76

The intercept C of about 5-10 $\mu g/m^3$ in Table 5.9 represents an approximately constant concentration of coarse particles. The slope of about 3 shows the scaling factor required to convert sulphate measurements to secondary PM_{10} on a network mean basis, this factor is required because the measurements are of sulphate only.

This relationship provides a method for illustrating the contributions to measured PM_{10} concentrations on a daily basis (Stedman, 1998). A constant coarse particle concentration is assumed for each day; the combustion related primary particle concentration is represented by the concentration of measured black smoke and the secondary particle concentration is estimated by multiplying the measured concentration of sulphate by a factor of three. This is partly determined by the relative locations of the PM_{10} black smoke and sulphate monitoring sites. While urban areas in England are strongly

represented in both the PM_{10} and black smoke monitoring networks, the sulphate monitoring network sites are more evenly distributed, with several sites in remote areas of Scotland and Northern Ireland (APEG, 1999). This is important because there is a gradient in particulate sulphate across the country, with concentrations in southern England being more than twice those are in northern Scotland (RGAR, 1997). Values in the range 2-2.5 are obtained if this factor is calculated on the individual site, rather than network mean basis. This method is used to predict PM_{10} level of the city. As ADMS_Urban can predict the PM_{10} from primary sources, contributions from coarse and secondary sources need to be added to gain the overall PM_{10} concentration.

Either black smoke measurements or oxides of nitrogen (NO_x) measurements are used as an indicator for primary combustion particles and rural sulphate measurements are used as an indicator for secondary particles (Stedman, 1998):

$$[measured\ PM_{10}] = A_{bs}\ [measured\ black\ smoke] + B\ [measured\ sulphate] + C$$

or

$$[measured\ PM_{10}] = A_{NOx}\ [measured\ NO_x] + B\ [measured\ sulphate] + C$$

5.4.5 ADMS_Urban Predicted PM_{10} and Imported PM_{10}

In the Leicester emissions database, only primary sources are included. PM_{10} is modelled by taking account of primary emission only. In short, ADMS_Urban can only model the primary part of the overall PM_{10} values. This is the main reason for the great under-prediction of PM_{10} by ADMS_Urban. It can be expected that if secondary sources

and coarse sources of PM_{10} are added to the ADMS_Urban predicted values, the total value will be scaled up to nearer the monitored values. The equation used is,

[measured PM_{10}] = ADMS modelled + 7.5 [measured sulphate] + Coarse

Background sites (See Figure 5.19) are chosen as following according to the wind direction;

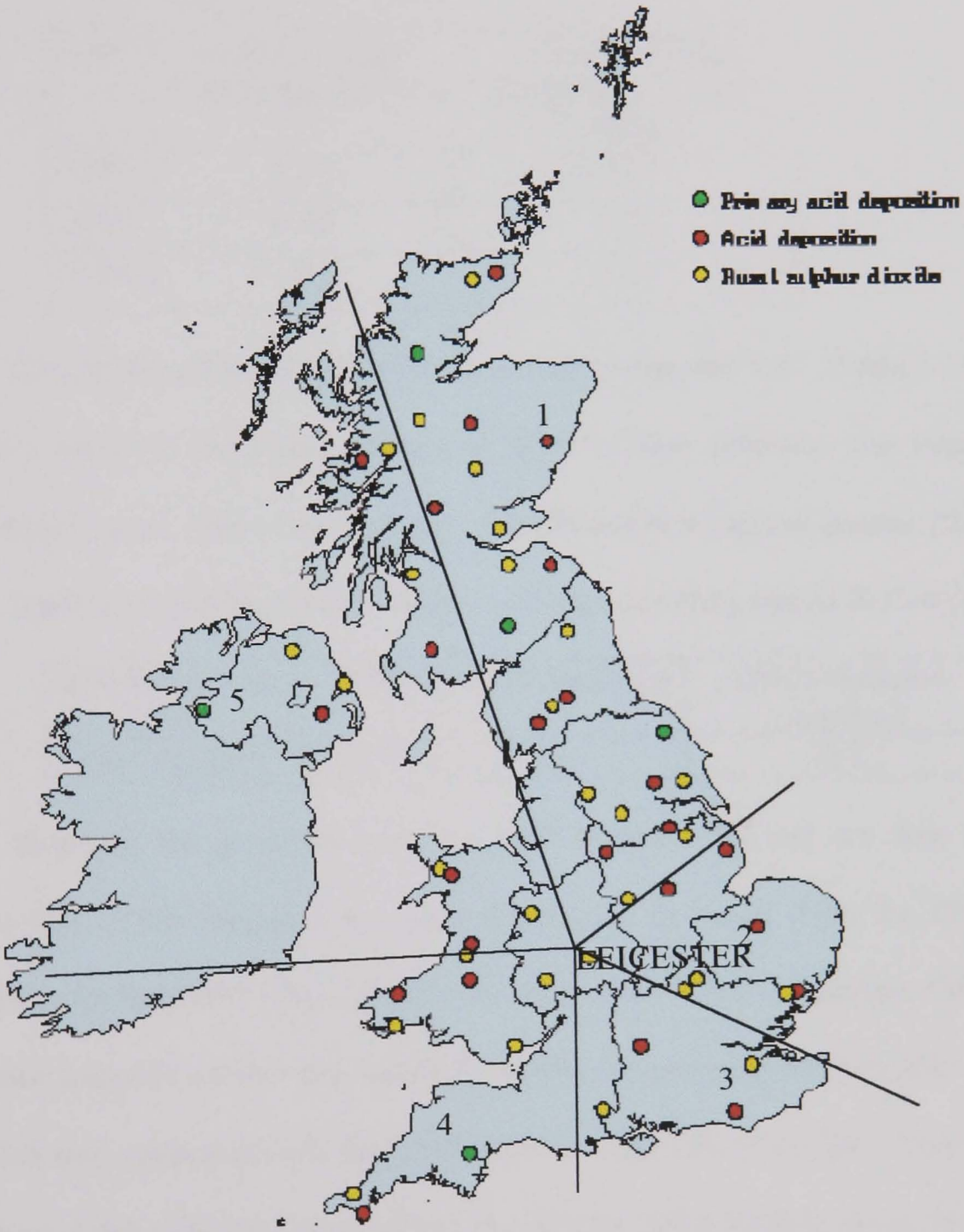
1. High Muffles (340- 45 degrees)
2. Stoke Ferry (45 - 120 degrees)
3. Barcombe Mills (120 - 180 degrees)
4. Yarner Wood (180 -260 degrees)
5. Lough Navar (260 - 340 degrees)

The measured sulphate data has been selected from the rural site High Muffles, Stock Ferry, Barcombe Mills, Yarner Wood and Lough Navar according to the wind directions. Sulphate particles, as mass of sulphur, are all expressed all in micrograms of per cubic metre. The value of coarse sources 5μg/m3 is chosen for Leicester as recommend by CERC (in the next release of ADMS_Urban, imported PM_{10} values will be taken into account by inputting from its newly designed interface[2]).

[2] Private communication with CERC.

Figure 5.19 PM_{10} Background Sites

(Background map from http://www.aeat.co.uk/netcen/airqual/index.html)



By employing the method described in section 5.4.2, the secondary and coarse PM_{10} annual average are as shown in Table 5.10. Therefore, ADMS_Urban prediction output plus imported values (secondary and coarse) can be compared with AUN data.

Table 5.10 Leicester Secondary and Coarse PM_{10} ($\mu g/m^3$)

Year	Annual Average Secondary PM_{10}	Annual Average Secondary + Coarse PM_{10}
1995	8.67	13.67
1996	8.32	13.32
1997	6.08	11.08

The ADMS_Urban predicted PM_{10} annual average for 1997 (Table 5.11) was only 7.1$\mu g/m^3$, however, the annual average of ADMS_Urban predicted plus imported PM_{10} reached 18.2 $\mu g/m^3$, which was very close to AUN monitored annual average 20.9$\mu g/m^3$.

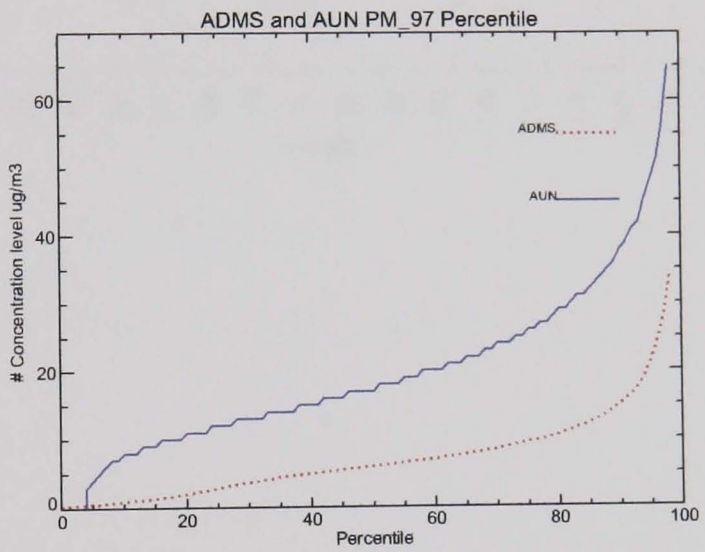
Table 5.11 ADMS_Urban Predicted and Imported PM_{10} and AUN Comparison

Annual Average (1997)	AUN	ADMS Predicted	ADMS Predicted +Imported
PM_{10} ($\mu g/m^3$)	20.9	7.1	18.2

Similarly, the percentile plots for 1997 (Figure 5.20) and raw time series plots (Figure 5.21, 5.22) suggested the same conclusion. In Figure 5.20, the first plot was repeated as for year 1997 when no imported values were added to compare with the second plot when imported values were added. By adding the secondary sources and coarse to the modelled data, comparing with the AUN monitored data, the percentile plots show a better agreement. After adding imported values, the ADMS_Urban predictions reached the similar level as AUN monitored values, though slightly over-predicted at lower percentiles, and slightly under-predicted at higher percentiles (Figure 5.20). By adding imported values, for

the period 1 February -7 February 1997 (Figure 5.21) and period 1 January - 28 Juanary 1997 (Figure 5.22), ADMS_Urban successfully predicted some AUN peak values too. The difference caused by the imported values being added to ADMS_Urban predictions can be clearly seen. ADMS_Urban performed well in predicting PM_{10} values by using this technique.

Figure 5.20 ADMS_Urban and AUN PM_{10} Percentile Analysis 1997



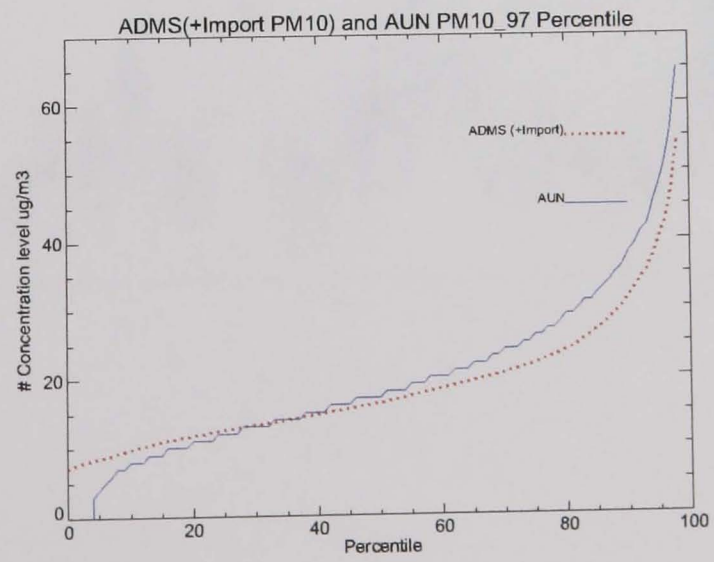
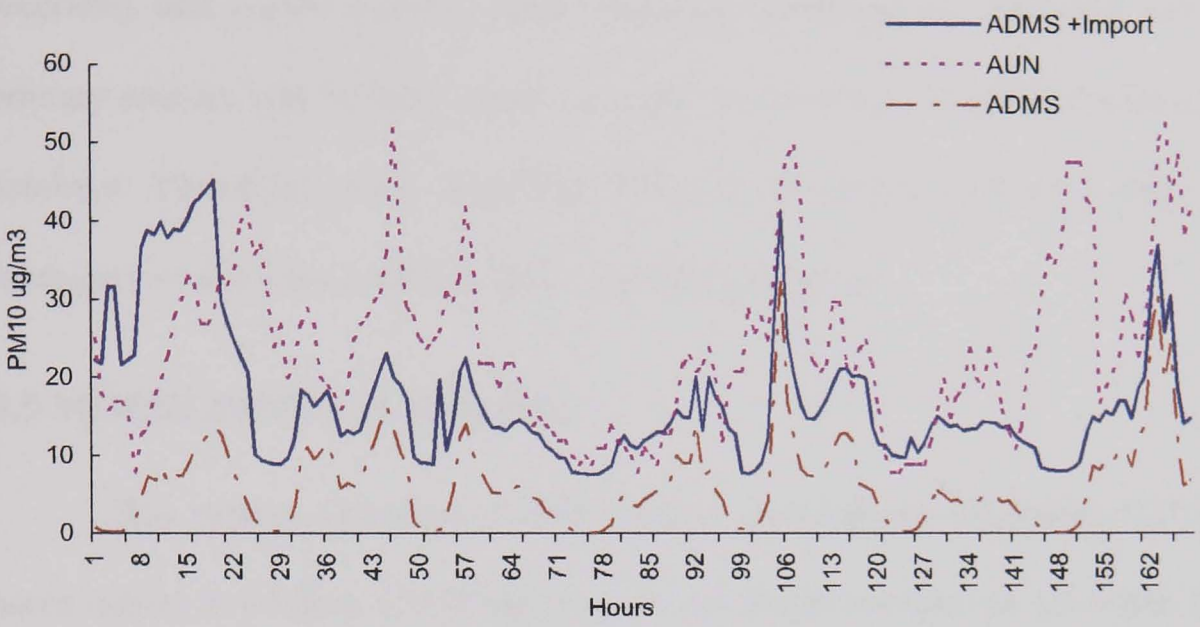
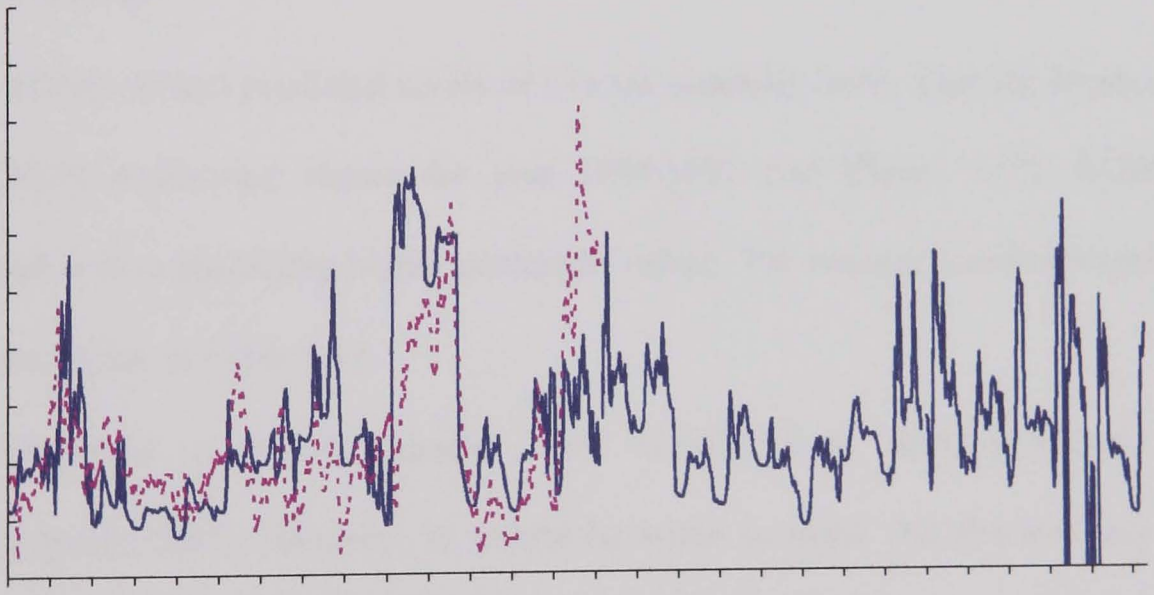


Figure 5.21 ADMS (+Import) and AUN PM10 1/2/97-7/2/97





5.4.6 Summary

As discussed in this section, ambient concentrations of PM_{10} arise from primary, secondary and coarse sources. Local emissions databases can normally only contain the primary sources and ADMS_Urban can only model what is contained within the emission database. Therefore, when modelling PM_{10}, it is vital to add the values which from secondary sources and coarse to gain a realistic prediction.

5.5 MODELLING CO AND SO_2

This section examines ADMS_Urban's performance predicting CO and SO_2. As noted earlier in Chapter 4, CO and SO_2 are not major concerns in Leicester. CO is mainly caused by traffic emissions. SO_2 is mainly from industrial point sources. ADMS_Urban predicted CO and SO_2 values are compared with monitored AUN values in this section.

5.5.1 Modelling CO

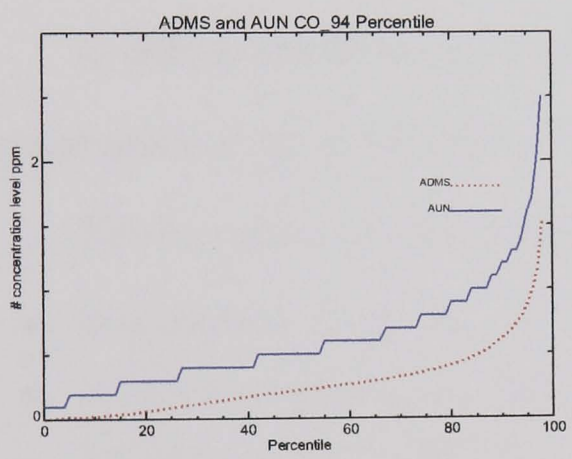
ADMS_Urban predicted levels of CO are generally lower than the levels measured at the AUN monitoring station for year 1994-1997 (see Figure 5.27). ADMS_Urban performed well at predicting higher percentile values. The average concentrations for each period are shown in Table 5.12.

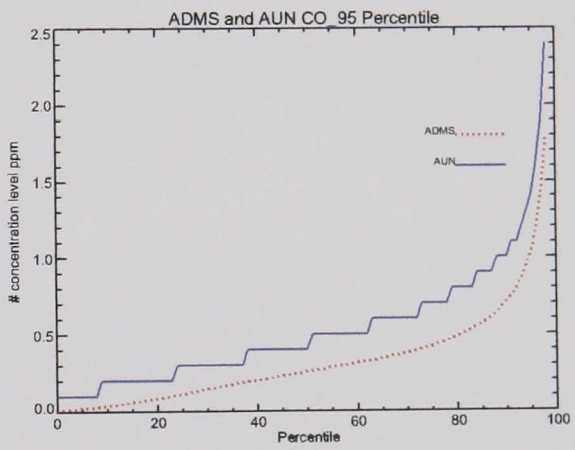
Generally it would appear that ADMS_Urban under-predicted CO by approx.0.2ppm (50%). However, it should be borne in mind that the accuracy of AUN measurement for CO is $\pm$8% and the precision of AUN measurement for CO is $\pm$ 0.6 ppm (AEA, 1998). ADMS_Urban predictions are therefore within the tolerances of monitoring equipment. So, the ADMS_Urban predicted values can be considered to be acceptable.

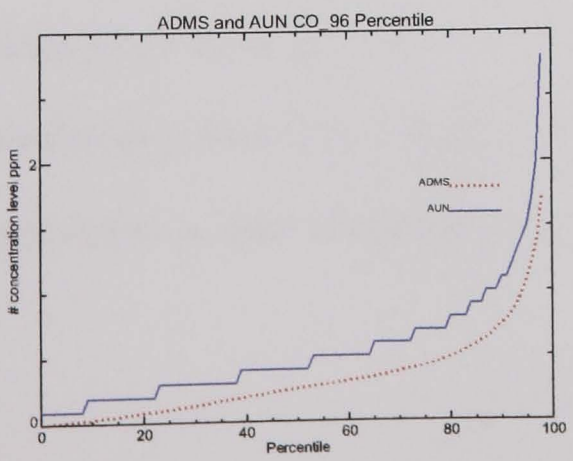
Table 5.12 CO: ADMS_Urban prediction and AUN data average comparison

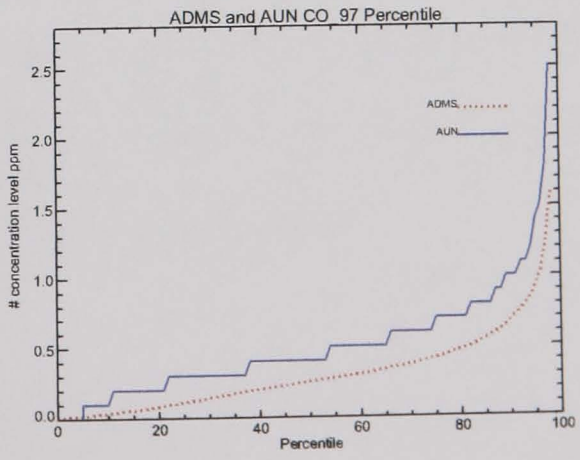
Year	AUN Annual Average (ppm)	ADMS Annual Average (ppm)	Percentage of under/over prediction	Correlation coefficient (hourly)
1994	0.62	0.27	-56%	0.51
1995	0.54	0.33	-39%	0.41
1996	0.55	0.33	-40%	0.47
1997	0.57	0.31	-46%	0.45

Figure 5.23 CO: ADMS_Urban Annual Output and AUN Data Percentile Comparison 1994 - 1997









5.5.2 Modelling SO_2

This section aims to test the performance of ADMS_Urban model to predict the SO_2 levels in Leicester. As noted earlier, SO_2 is generally considered not to be a problem in Leicester, but occasionally, some high levels are recorded. SO_2 is mainly from industrial point sources, so episodes are generally likely to be related to local wind conditions. Therefore, SO_2 episodes in Leicester are analysed first, then the annual (1994-1997) and monthly (August 1996, December 1996, and January 1997) predictions are followed using the same procedure as for NO_2, NOx and PM_{10}.

SO_2 Episode

In order to identify the relationship between SO_2 episodes and wind conditions, the probability of occurrence of high SO_2 values were examined.

The data sets used in this analysis were:

- SO_2 data from AUN 1994, AUN 1997 and LAMS 1997
- 1994 Meteorological data from Birmingham Elmdon station
- 1997 Meteorological data from Leicester Meteorological Mast, January-September

Analysis of SO_2 episodes and meteorological data (Figure 5.24, Figure 5.25) shows that the peak level SO_2 concentrations mostly occurred at low wind speeds and under non-prevailing wind direction conditions. The results from the simple plots and the polar plots agree each other. It is worth investigating the distribution of SO_2 emission sources in Leicester and the relationships between the emission sources, the concentrations and the meteorological conditions. The local meteorological data will be analysed to see if there are any promises in order to identify the main sources and the main effects.

The probability of occurrence polar plots show the peak level SO_2 concentrations are mainly distributed at the non-prevailing wind direction for 1994 (North-east) and 1997 (north-west) at AUN site (Figure5.24, Figure5.25). However at the LAMS site, the plots show a slightly different pattern (Figure5.26), the peak levels of SO2 were most likely to occur when winds were from the North-west, then secondly likely to occur when winds were from south-west. .

Analysis of SO_2 episodes and wind direction showed

- The main wind direction was 150-250 degrees
- SO_2 peak levels were mostly distributed at non-prevailing wind direction, and low wind speed.

In terms of the location of power stations to the north of Leicester, the peak level SO_2 could possibly occur when the wind was from North (non-prevailing wind direction), however the main wind direction was from south-west (Figure 5.17). SO_2 levels at the LAMS station might be effected by a local source (e.g. boiler in a school nearby). It was also possible that high level SO_2 was from the Birstall area (immediately North of the city) where some coal burnings may still take place.

Annual SO_2 prediction and Analysis

ADMS_Urban annual scenarios for SO_2 from 1994 to 1997 were calculated. ADMS_Urban considerably under-predicts SO_2 levels (Figure 5.27). This is because sources were not fully incorporated in the emission database, because at the term of its preparation SO_2 was not considered to be a priority for investigation by Leicester City

Council[1]. This means that there is little point in trying to validate SO_2 predictions in absolute terms.

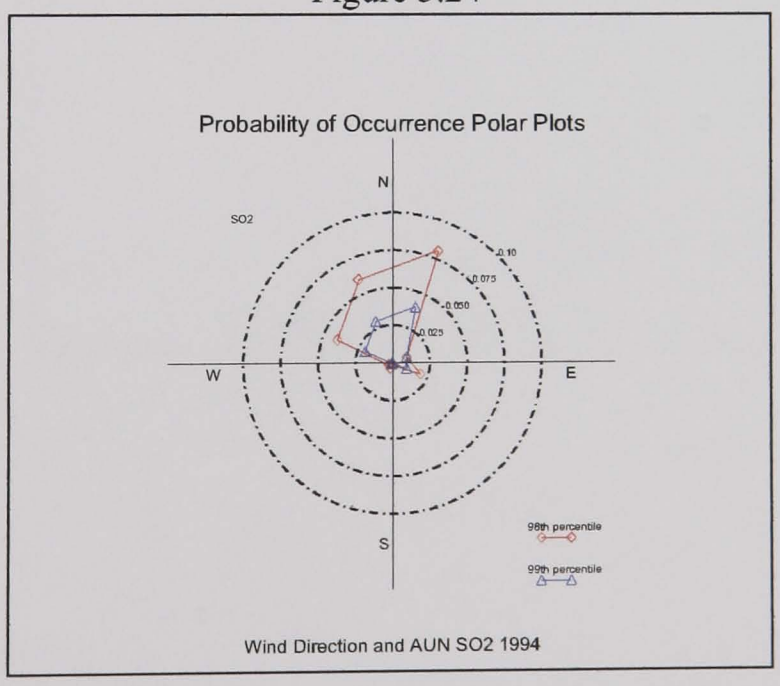
Monthly SO_2 Prediction and Analysis

The percentile plots (Figure 5.28) showed that ADMS_Urban predicted levels of SO_2 were lower than the levels measured at the AUN station. However, ADMS_Urban high percentile level was higher than measured level for August 1996 and December 1996. The average concentrations for each period are shown in Table 5.13. The reason for this is explained in the precious section.

Table 5.13 SO_2 : ADMS_Urban output and AUN data average comparison

Code	AUN Average (ppb)	ADMS Average (ppb)	Percentage of under/over prediction	Correlation coefficient
9608	4.25	1.47	-65%	0.18
9612	5.7	0.91	-84%	-0.06
9701	5.48	0.78	-86%	-0.01

Figure 5.24



[1] Private communication with LCC.

Figure 5.25

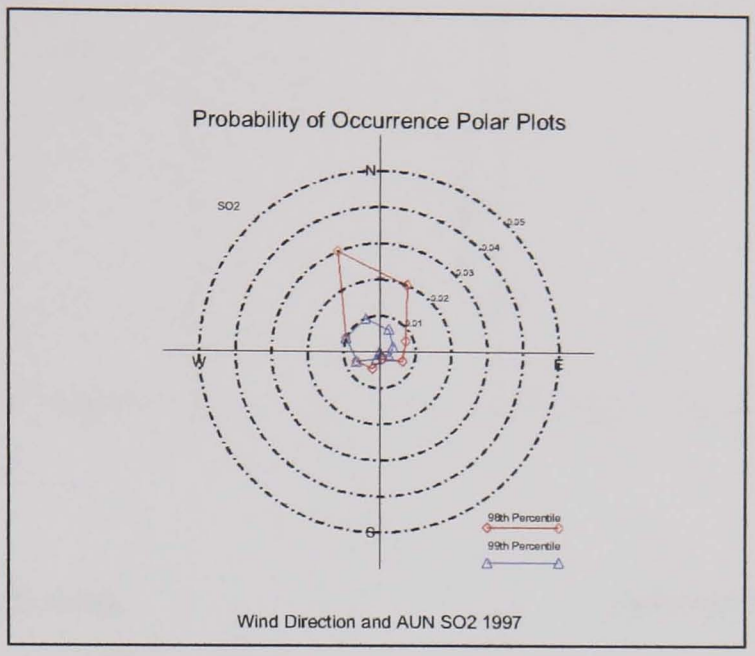


Figure 5.26

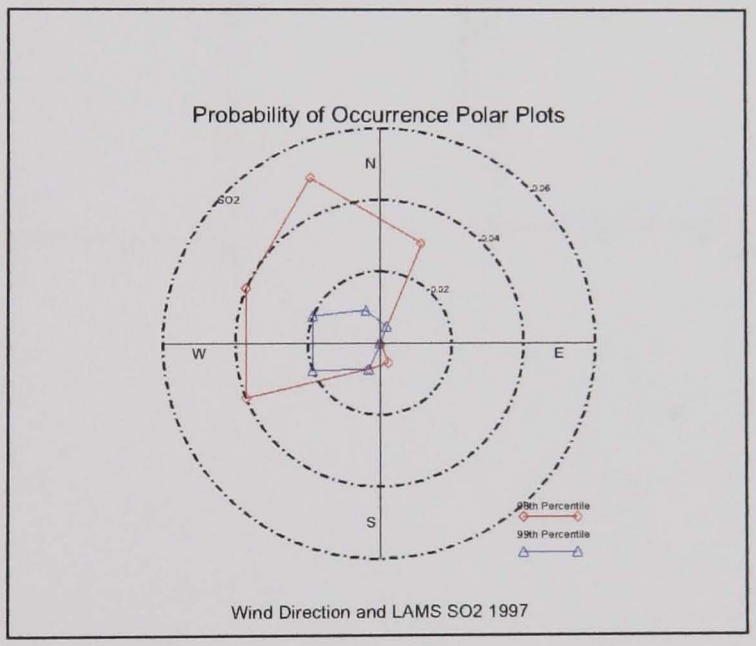
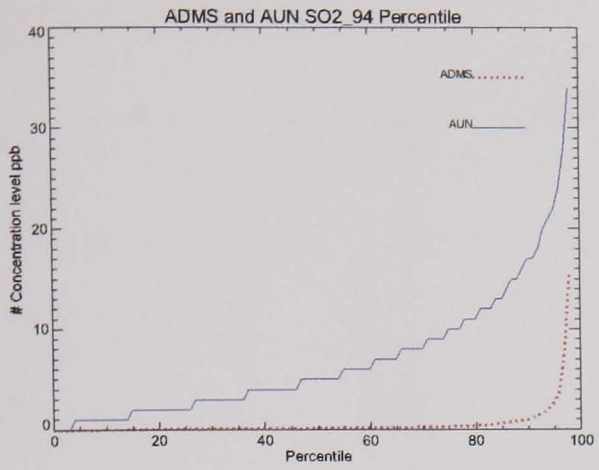
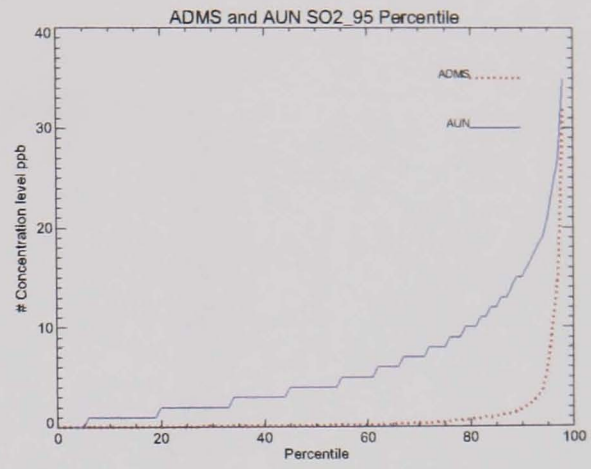
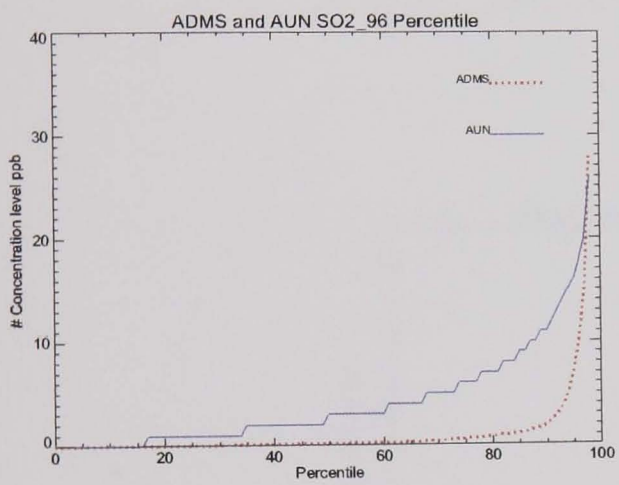


Figure 5.27 SO_2: ADMS_Urban Annual Output and AUN Data Comparison







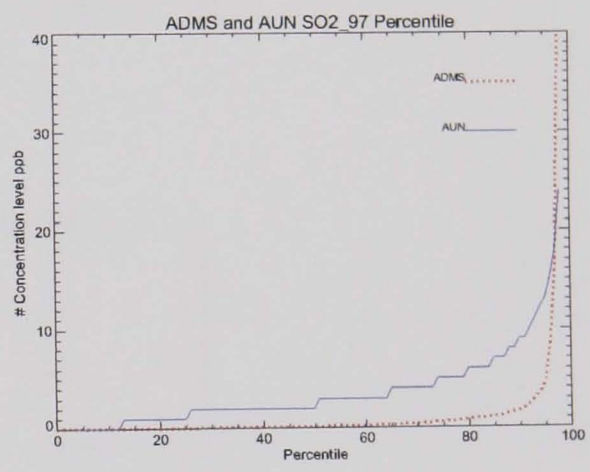
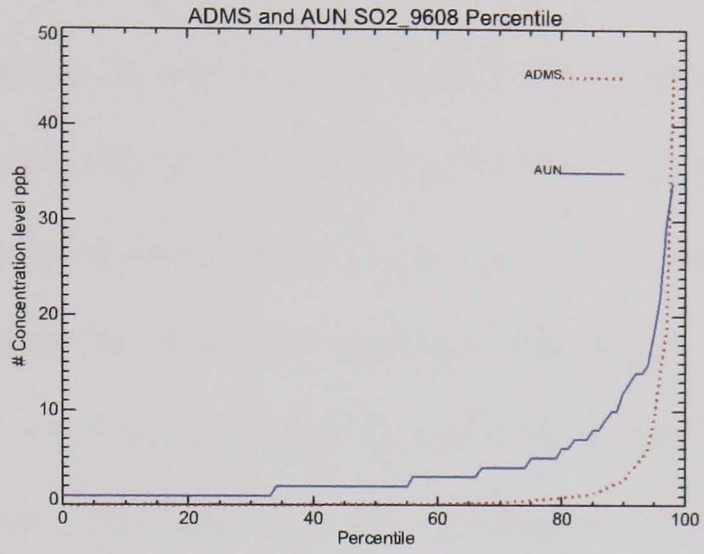
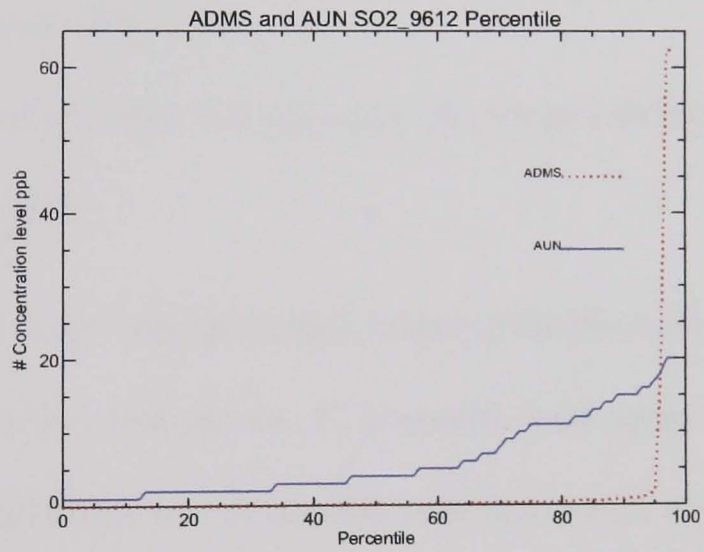
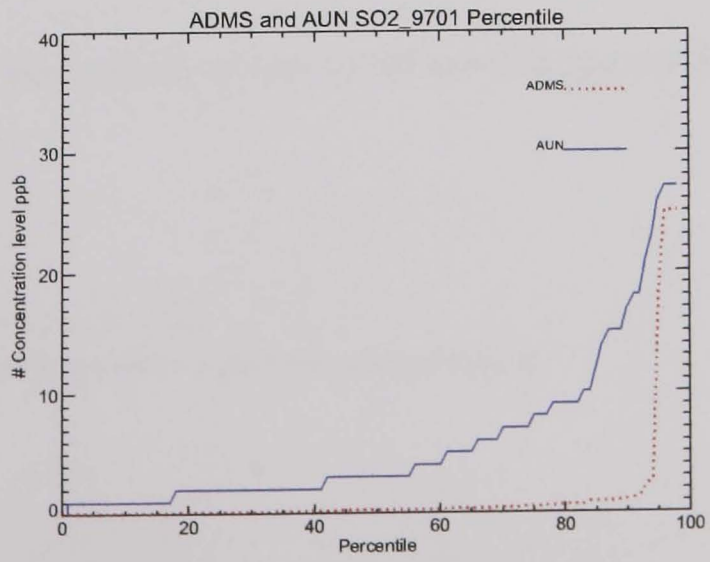


Figure 5.28 SO_2 : ADMS_Urban Output and AUN Data Percentile Analysis







5.6 USE OF LOCAL METEOROLOGICAL DATA

As noted earlier, the parameters monitored at the Leicester Meteorological Mast include temperature at 2m and 10m above ground level, wind direction at 10m, wind speed at 10m, standard deviation of the horizontal wind direction (derived), standard deviation of the vertical wind speed (derived). As cloud cover is not available, the surface heat flux needs to be calculated based on the temperature difference at 2m and 10m. Therefore, heat flux, wind speed, wind direction and temperature can be inputted to ADMS_Urban to meet the basic input data requirement (also refer to Chapter 3, section 3.2.2). Surface heat flux represents the radiant heat transfer rate between air and earth surface.

5.6.1 Calculation of Heat Flux

The surface heat flux H is defined as (Panofsky and Dutton, 1984)

$$H = C_p \rho \overline{W'T'} \qquad (5\text{-}1)$$

Where W' and T' are the surface values of the fluctuating components of the vertical wind and temperature, respectively. C_p is specific heat capacity of air and ρ is air density. The heat flux calculated here is sensible heat flux which is generally proportional to the vertical temperature gradient. Described below is the methodology used for calculating surface heat flux[1]. Calculation of heat flux from measurements of average temperatures at two heights and wind velocity at one (or different) height are discussed in this section.

[1] CERC assisted with the method to calculate surface heat flux.

Methods are based on the assumption of constant vertical fluxes of momentum and heat near the surface. Such assumptions can be questionable near the surface in urban areas. Panofsky and Dutton (1984) derived an expression for the heat flux H as

$$H = \frac{-\rho c_p \kappa^2 U(z_3)(\theta(z_2)-\theta(z_1))}{\left[ln\left(\frac{z_3}{z_0}\right)-\psi_{m_3}\right]\left[ln\left(\frac{z_2}{z_1}\right)-\psi_{\theta_2}+\psi_{\theta_1}\right]} \tag{5-2}$$

where ψ_{m_3} is related to the non-dimensional wind shear at $z_3, \phi_m(z_3)$, and $\psi_{\phi_2}, \psi_{\phi_1}$ are related to the temperature gradients $\phi_\theta(z_1)$ and $\phi_\theta(z_2)$ at heights z_1 and z_2.

In stable flows, ψ_{m_3} is expressed as

$$\psi_m(z) = -5\frac{z}{L} \tag{5-3}$$

$$\psi_\theta(z) = \psi_m(z) \tag{5-4}$$

In convective flows, ψ_m and ψ_θ are expressed as

$$\psi_m = \ell n\left[\left(\frac{1+x^2}{2}\right)\left(\frac{1+x}{2}\right)^2\right] - 2\tan^{-1}(x) + \frac{\pi}{2} \tag{5-5}$$

$$\psi_\theta = 2\ell n\left[\frac{1}{2}\left(1+\left(1-16\frac{z}{L}\right)^{\frac{1}{2}}\right)\right] = 2\ell n\left(\frac{1}{2}\left(1+x^2\right)\right) \tag{5-6}$$

where $x = \left(1-16\frac{z}{L}\right)^{\frac{1}{4}}$

Note that, here,

$$\theta(z_2)-\theta(z_1) = T(z_2)-T(z_1)+\gamma_d(z_2)-\gamma_d(z_1)$$

$$= T(z_2) - T(z_1) + \gamma_d (z_2 - z_1) \qquad (5\text{-}7)$$

where γ_d is the dry adiabatic lapse rate ~ 10^{-2} Cm^{-1}. (This could be modified in saturated conditions.)

Monin-Obukhov length L is expressed as

$$L = \frac{-u_*^3 c_p \rho T}{\kappa_g H} \quad \text{Monin-Obukhov length} \qquad (5\text{-}8)$$

Where

$\theta(z)$	Mean potential temperature at height z (for relationship to temperature T) See (5-7)
ρ	Deviating air
C_p	Specific heat capacity of air
κ	Von Karman' s constant (~0-4)
$U(z)$	Mean wind speed at height z
H	Heat flux

In unstable conditions, only the following heat flux calculations use the first approximation to heat flux, i.e. the equation is,

$$H(\theta_0) = \frac{-\rho c_p \kappa^2 u(z_3)(\theta(z_2) - \theta(z_1))}{\ln(z_3 / z_0) \ln(z_2 / z_1)} \qquad (5\text{-}8)$$

where,

ρ = density of air (1.225 kg/m^3)

c_p = Specific heat capacity of air (1012 $J/^0C/kg$)

κ = Von Karman' s constant (0.4)

u(z) = wind speed at height z

$\theta(z)$ = potential temperature at height z

z_3 = height of wind speed measurement (10m)

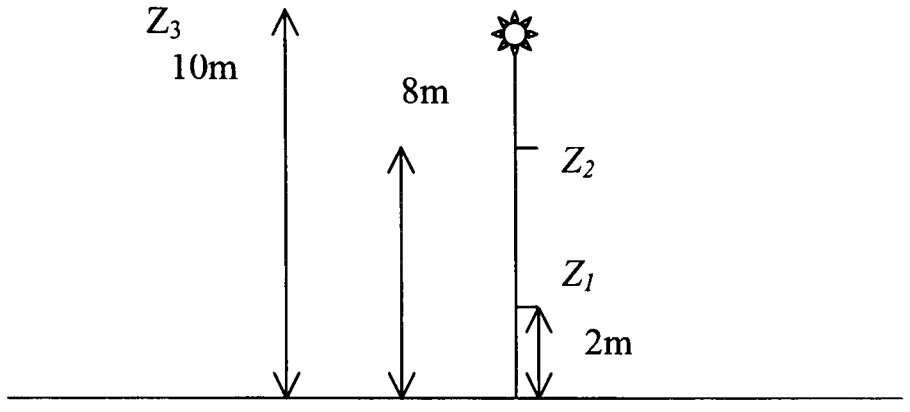
z_2 = upper temperature measurement (8m)

z_1 = lower temperature measurement (2m)

z_0 = roughness length (0.3m)

An illustration of measurements is shown in Figure 5.33.

Figure 5.29 Illustration of Meteorological Mast Measurements



5.6.2 Method to calculate heat flux

As known in meteorological data

z_3 = 10m z_3 is wind speed height.

z_1 = 2m, z_2 = 8m z_1 and z_2 are temperature measurement height.

The calculating steps to follow are as,

(i) Calculate H assuming neutral flow $\frac{1}{L}$ tends to infinity

(ii) Calculate L using equation (5-7)

(iii) Calculate U using

$$U(z)=\frac{u^*}{\kappa}\ell n\left(\frac{z}{z_0}+\psi_m\left(\frac{z}{L}\right)\right) \qquad (z = 10\text{m}) \qquad (5\text{-}10)$$

Note here x will be derived from equation (5-3) or equation (5-4) depending on whether it is stable or unstable conditions, while $\theta(z_2)>\theta(z_1)$ or $\theta(z_2)<\theta(z_1)$.

Where $\theta(z_2) > \theta(z_1)$, the equation in stable condition is used.

In unstable condition, $\theta(z_2) < \theta(z_1)$, equation (5-8) is used.

Then repeat (i) to (iii) steps and, no longer assuming that $\frac{1}{L}$ tends to infinity until the condition is fulfilled when the gap between final iteration and the last iteration is less than 5 watt/m^2. This is an iterative method.

5.6.3 Results comparing with Elmdon heat flux

Heat flux calculated for the Leicester Meteorological Mast using the above equations are considered in this section. Results for two winter months (February and March) and summer months (July and August) are shown (Figure 5.30 to Figure 5.33). These plots show the comparison between the calculated heat flux for Leicester and the heat flux values derived by ADMS_Urban meteorological pre-processing module for Elmdon. A good agreement between calculated heat flux for Leicester and the measured values at Elmdon can be found. It can be seen that in winter months (Figure 5.30 and 5.31), the peak values of heat flux were mostly below 100 watt/m^2, rarely reached 200 watt/m^2, and the average values at Elmdon station 25.2 watt/m^2 and Leicester station 20.7 watt/m^2 were in good agreement. Positive values represent heat transfers towards earth surface, and negative values represents heat transfers to opposite earth surface. During the daytime, surface heat flux is likely to be positive.

Figure 5.30 Heat Flux in February 1997

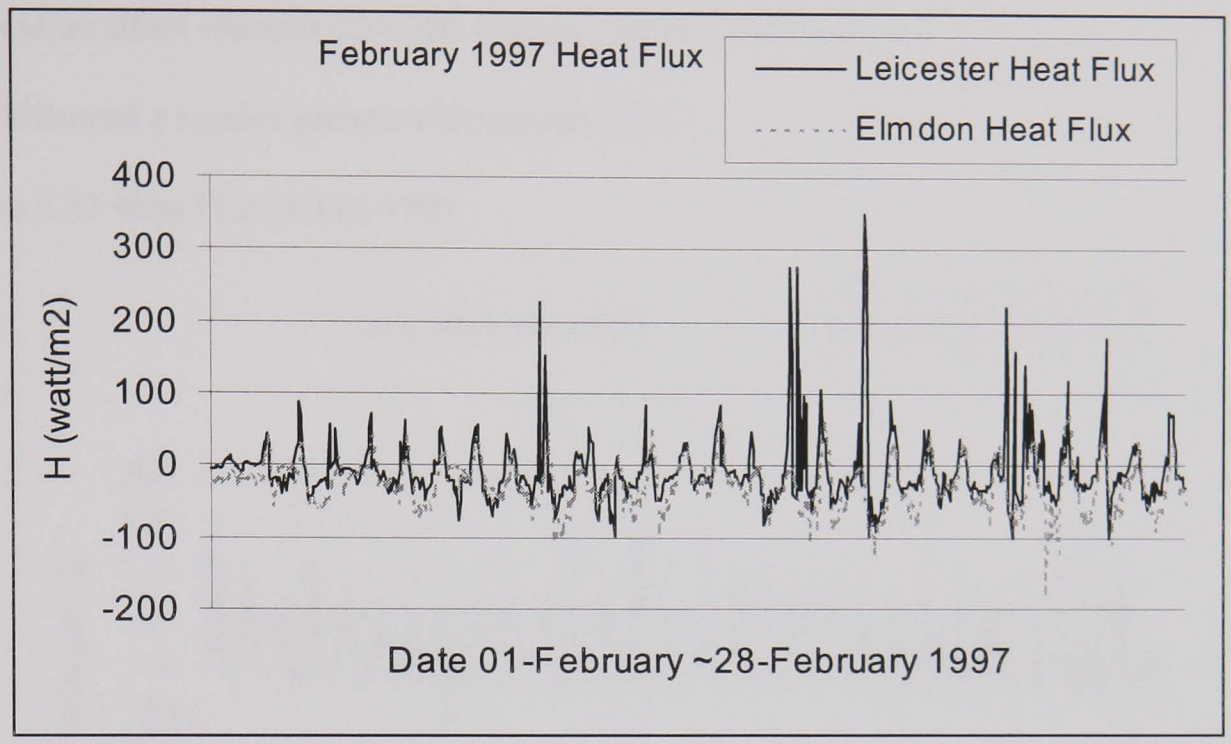
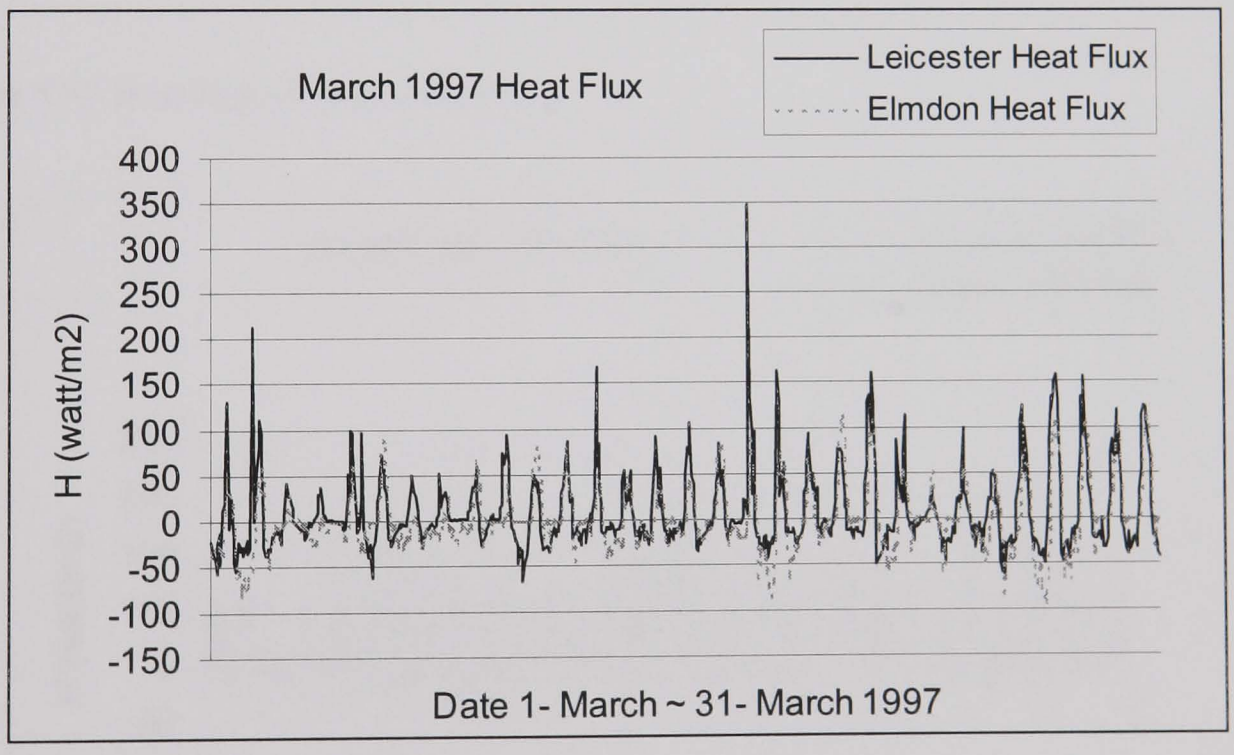


Figure 5.31 Heat Flux in March 1997



The heat flux values of summer months can be seen from Figure 5.32 and 5.33, heat flux values often reached 100-150 watt/m^2, and the average value at Elmdon and Leicester both followed a similar pattern with similar levels.

Figure 5.32 Heat Flux in July 1997

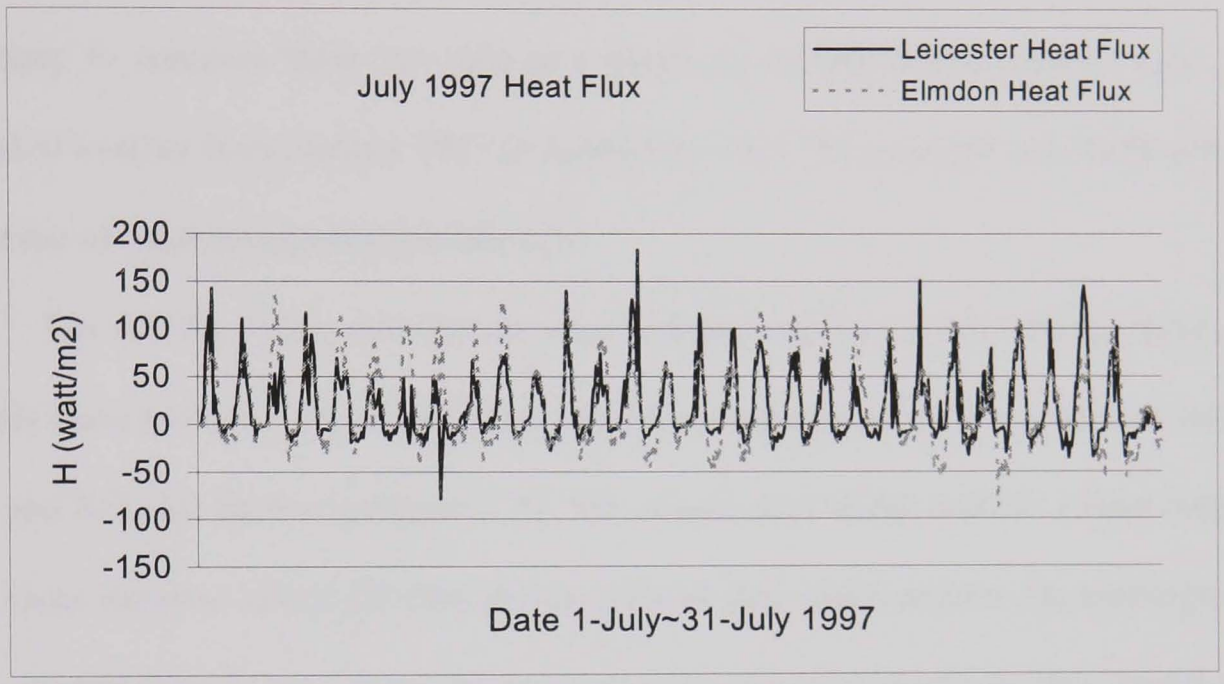
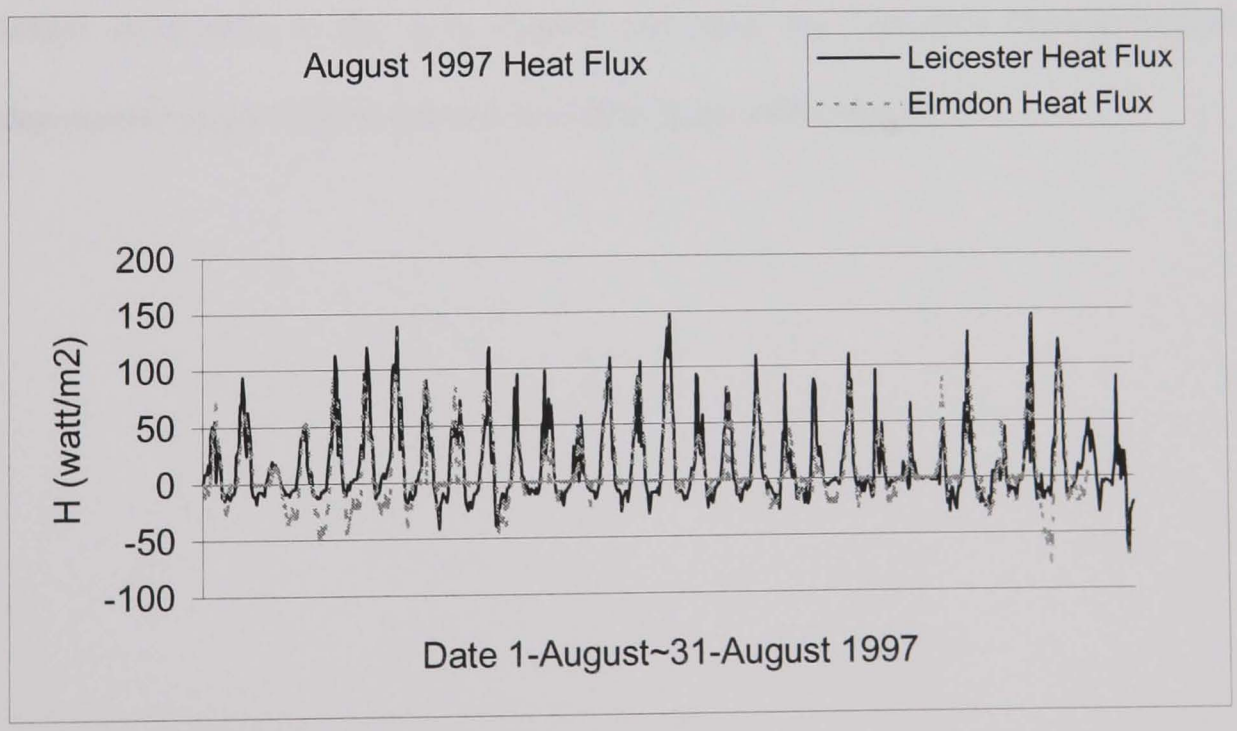


Figure 5.33 Heat Flux in August 1997

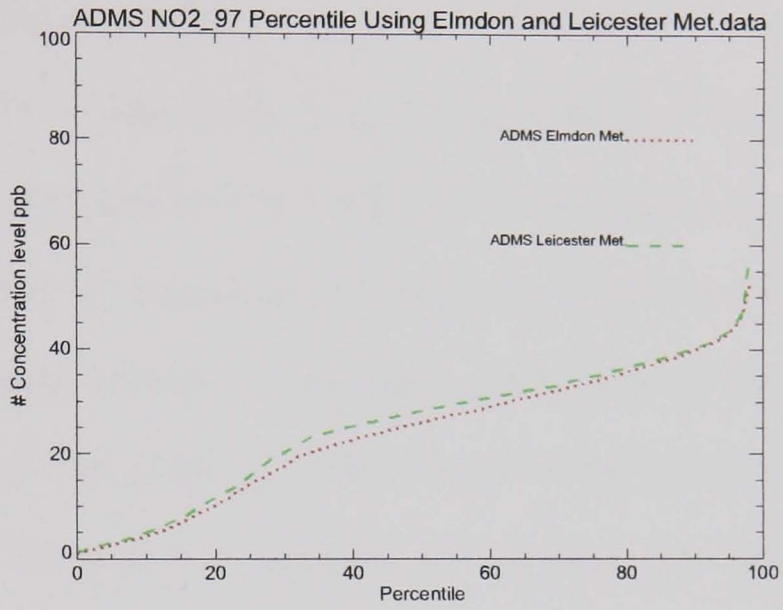


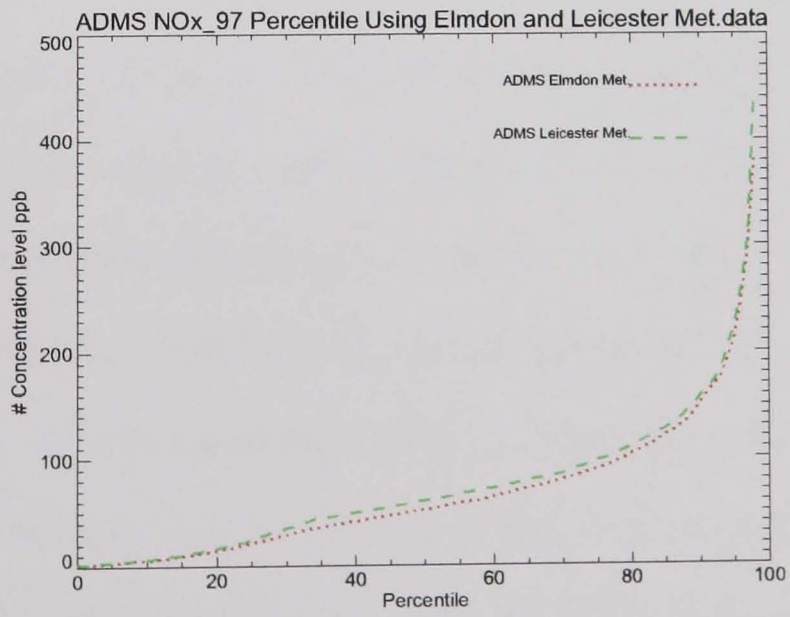
As heat flux is one of the most important parameters for pollution dispersion, these findings indicate that the Leicester Meteorological Mast and Elmdon station data should give very similar results using the ADMS_Urban model. The calculated surface heat flux in Leicester served as one of input meteorological parameters for ADMS_Urban. It is necessary to compare these two data sets based on ADMS_Urban model output for the period of overlay from January 1997 to September 1997. This comparison lends confidence to the use of local meteorological data sets.

The ADMS_Urban simulations using both meteorological data sets for these overlap periods therefore were examined. The percentile comparison of the modelled values for NO_2 and NO_x are shown in Figure 5.34. The results proved the ADMS_Urban outputs are very close between using Elmdon Meteorological data and Leicester Meteorological data with calculated heat flux. It can be concluded that the calculated heat flux from Leicester meteorological data is suitable for input. Subsequently, the 1998 meteorological data used for further simulation in the next chapter was from the Leicester Meteorological Mast (Elmdon meteorological data was not available from 1998 onwards).

Figure 5.34 ADMS Output Percentile Comparison using Elmdon and Leicester Meteorological Data

(January -October 1997)





5.7 SUMMARY

In this chapter, comparisons of ADMS_Urban predictions for a range of pollutants with AUN monitored data were undertaken.

For NO_2, modelled and monitored values show reasonable agreement. The accuracy of predicted annual mean NO_2 levels were of the order of -23% (1997) to just +1% (1994). ADMS_Urban successfully predicted some NO_2 and NOx peak levels. However, it failed to predict the peak level or pollution incident simultaneously, especially for NOx peak levels. Despite the instantaneous prediction being poor, overall, the model provides a standard of prediction that can be considered acceptable for the purposes of local air quality management. The GRS chemistry model used in ADMS_Urban to predict O_3, NO_2 and NOx values was also examined. Imported 1997 national remote Ozone background values for Leicester, national remote O_3, NO_2 and NO_x background values for Leicester, Leicester AUN O_3 background respectively were utilised in the GRS scheme. The results indicate that predictions can be improved by taking remote NO_2, NOx and O_3 values into the simulation.

ADMS_Urban predicted levels of PM_{10} are consistently lower than the levels measured at the AUN monitoring station. By examining various PM_{10} episodes crossing the country, it was shown that such episodes are national wide. In examining the modelling of PM_{10}, it was found that ADMS_Urban can only predict the PM_{10} from primary sources contained in the Leicester emissions database. Contributions from coarse and secondary sources need to be added to gain the overall PM_{10} concentration. It was shown that if secondary sources and coarse sources of PM_{10} are added to the ADMS_Urban predicted

values, the calculated total values compare more favourably with monitored levels. A good agreement between predicted PM_{10} and monitored PM_{10} can then be expected.

ADMS_Urban predicted levels of CO are generally lower than the (relatively low) levels measured at the AUN monitoring station in Leicester. However, ADMS_Urban model predictions are within the tolerances of monitoring equipment ($\pm$0.6ppm). Therefore, the ADMS_Urban predicted values for CO can be considered acceptable.

ADMS_Urban under-predicted SO_2 in Leicester. The cause of under-prediction is primarily due to the under-representation of SO_2 sources in Leicester's emission inventory. According to the analysis of SO_2 episodes and meteorological data, the peak level SO_2 concentrations almost occurred at the low wind speed and under non-prevailing wind direction conditions.

The use of Leicester Meteorological Mast data has been examined in this chapter. As the Birmingham Elmdon meteorological station was closed down at the end of 1997, the use of Leicester Meteorological data became necessary. A method of calculating the surface heat flux from data collected by the Leicester Meteorological Mast is presented. For the overlap period January 1997 to October 1997 ADMS_Urban simulations using Elmdon and Leicester meteorological data were compared. This showed good agreement between the two data sets, and provides confidence in the use of Leicester 1998 Meteorological Mast data for further modelling study in the following chapter.

CHAPTER 6 APPLICATION OF ADMS_URBAN - VALIDATION II AND STRATEGIC MODELLING

6.1 INTRODUCTION

In this chapter, sensitivity tests and strategic modelling are presented. The comparisons previously were made mainly for the AUN site. As one site may not be representative for whole urban area, ADMS_Urban predictions at monitoring stations other than the AUN (e.g. roadside air quality monitors) are undertaken here. The sensitivity of ADMS_Urban predictions in relation to the location of receptor points, close to the major roads, such as Melton Road and Welford Road, are analysed. Finally, the sensitivity of predictions to variation in vehicle speed are examined at Welford Road.

One of the major applications of air dispersion models is to aid urban planning by providing a means to predict the future air quality. The Environment Act 1995 requires every local authority to periodically review and assess air quality in its area. The primary purpose of this review and assessment is to determine whether the air quality objectives contained in the Air Quality Regulations 1997 are likely to be achieved by the end of 2005. In the majority of cases the review and assessment will need to include an assessment of likely traffic growth. The impact of traffic in Leicester for 2005 has been assessed using ADMS_Urban. This is referred to as "strategic modelling". For an overview of the pollution

distribution in the city, ADMS_Urban spatial outputs are included for 2005. A future traffic scenario at Belgrave Corridor is also presented in this chapter.

6.2 SENSITIVITY TESTS FOR AUN

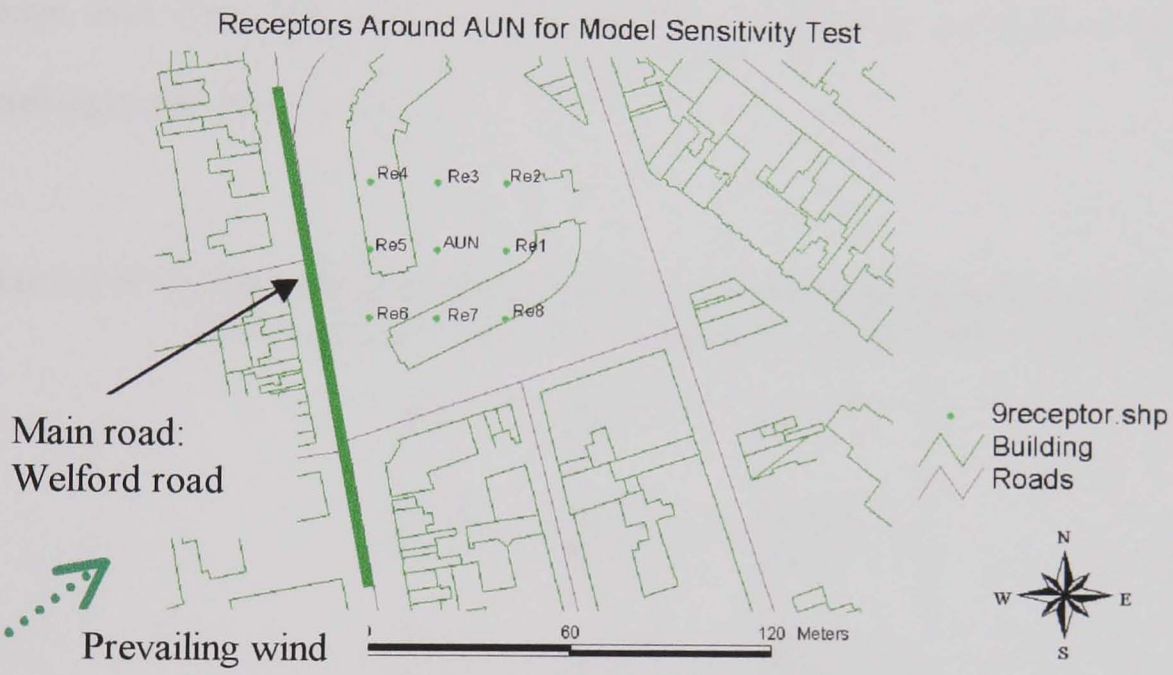
As reviewed in chapter 2, performing sensitivity analyses can quantify the response of a model in input parameter variation. Some input parameters account for the greatest sensitivity in the modelling output, these need to be identified so that appropriate care and attention is given to these at the preparation stage. Sensitivity tests also provide a view of what to expect for model output in conditions for which validation data is not available. An example of this technique is to systematically vary one or more of the input parameters to determine the effect on the modelling result. Results from sensitivity analysis therefore can provide useful guidance. Some input parameters and also the spatial sensitivity of model output are analysed in this section.

6.2.1 Receptor Grid at AUN Location

It was noted earlier that plume model can give rise to large pollution gradients over small spatial scales, so it is important to test the geometric accuracy of the model as the points being simulated can be located at various conditions such as near to a road, besides a building. This test looks at how much the modelled values at one receptor point would vary in relation to its specific location and its surrounding locations. In order to test the model spatial sensitivity for the AUN site, 8 receptors on a 20m grid around the AUN site were chosen. ADMS_Urban was used to obtain hourly predictions for NO_2 for the period from 1st August 1996 to 31st August 1996. Prevailing wind direction for this period was from

South-west. This period was chosen at random as a typical period without exceptional pollution incidents. The geographic distribution of these eight receptors is shown in Figure 6.1. It should be noted that buildings are not explicitly modelled in this simulation so receptor points may be superposed on a building footprint.

Figure 6.1 Receptors Distribution for Model Sensitivity Test



The results can be found in Table 6.1. The average value of nine receptors including receptor AUN is also shown under this table. The average modelled NO_2 value was greater than the AUN measured value. Re6 modelled value was grater than the value of Re5, so as Re5 modelled value was greater than Re4 value, similar patterns can be found from Re7 to Re 3, Re 8 to Re 2. The gradients in results were related to wind direction. As the prevailing wind direction was from the south-west, pollutant concentration dispersed along this direction. The predicted values of Re6, Re7 and Re8 were much greater. This was also due

to these receptor points were close to the busy road- Welford road as a major line source. Comparing the AUN monitored data and the average of eight receptors modelled data and the average of AUN receptor modelled data, it shows the modelled value at receptor AUN is the closest to the AUN measures values. In which case, it would appear that the AUN receptor point was correctly positioned relative to nearby emission sources. The test has demonstrated that large pollution gradients are predicted, with NO2 levels varying by 40ppb change over 40m. Therefore, it is important to identify the location of receptors when preparing model simulations.

Table 6.1 NO_2: Receptors at different directions 20 meters grid around AUN site
ADMS_Urban Predicted Average (ppb) (01/08/1996 - 31/08/1996)

Re 4 9.16	Re 3 10.07	Re 2 11.63
Re 5 24.51	Re AUN 21.04	Re1 18.70
Re 6 40.06	Re 7 48.25	Re 8 46.76

Average
25.58

AUN
monitored
20.80

Prevailing wind direction

6.2.2 Roadside Predictions

As noted from previous results, the prediction values immediately adjacent to a busy road are often higher than those in adjoining pedestrian areas. Vehicle speed will be shown to be one of the most important input parameters. In terms of roadside prediction, spatial grid analysis at Welford Road is also presented.

Vehicle speeds

Vehicle speeds are assumed to be constant over one road link in ADMS_Urban. However, in reality, during peak flow periods vehicle speeds will reduce and net emissions will therefore be increased. Presently the model only allows for the increase in net emission resulting from increased vehicle flow, not for the attendant decrease in vehicle speeds.

Vehicle speed is closely related to how much emissions are produced from road traffic. Designed Manual for Road and Bridge (DMRB, 1996) emission factors used in ADMS_Urban are for driving cycles based on an average speed. Other factors may be derived using a different criterion. To test the sensitivity of prediction to a wholesale change in vehicle speed, all the traffic speeds in the emission database were manually increased 5 km/hr. Welford Road, a busy road has been chosen for this test, as it is the closest road to AUN monitoring station. Meteorological data used was from Birmingham Elmdon for the month June 1994. A significant change can be seen in Figures 6.2 and 6.3 with regard to predicted values. As vehicle speed increased 5 km/hr in general, the predicted NO_2 and NOx values are also increased, particularly for the peak levels. Time series plots of modelled NO_2, NO_x levels under these changed conditions have been plotted

(Figure 6.2 and Figure 6.3). The outputs show that the ADMS_Urban modelled values are particularly sensitive to input vehicle speed. Therefore it is important to characterise the vehicle speed as accurately as possible in the emission database, given the inherent limitation of fixed vehicle speed along the same road link in ADMS_Urban.

Figure 6.2 Welford Road NO_2 Prediction for Changed Vehicle Speed

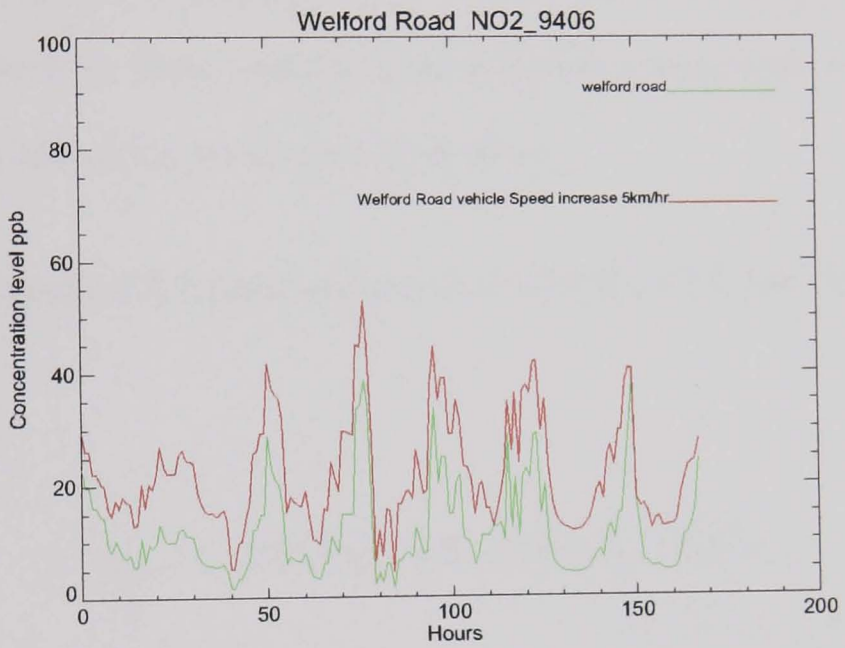
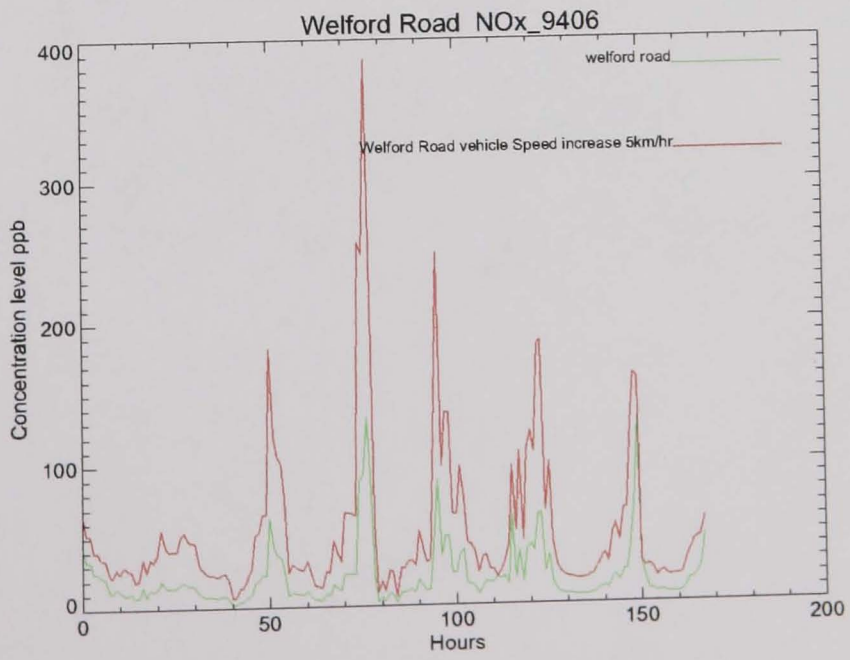


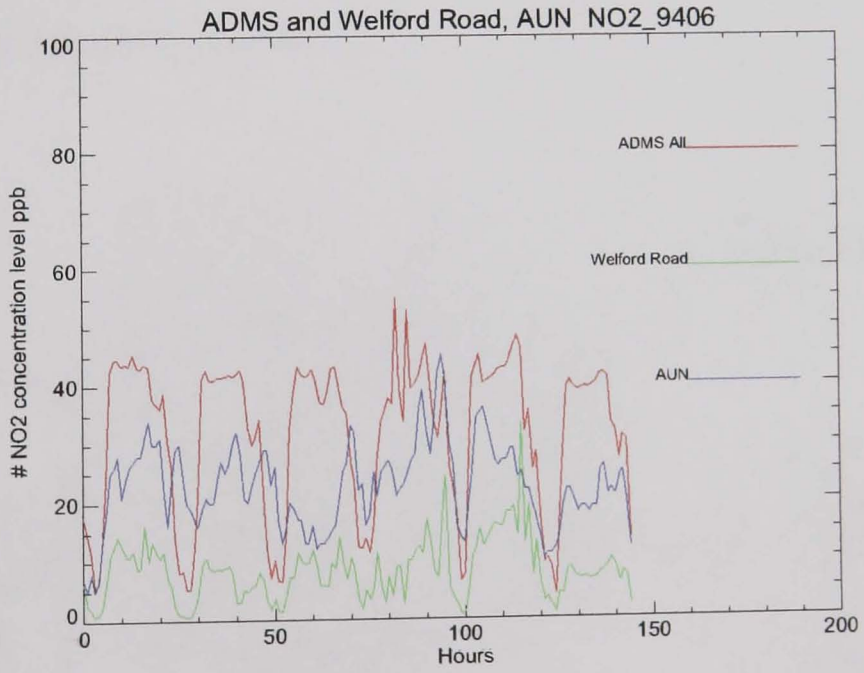
Figure 6.3 Welford Road NO_x Prediction for Changed Vehicle Speed



Pollution contribution of a busy road

In order to identify how much contribution the nearest road can make to (predicted) AUN receptor concentration level, modelled NO_2 concentrations were compared with AUN data and also with modelled NO_2 concentrations only from Welford Road for the period of June 1994. The monitored AUN values are also plotted. It was found that ADMS_Urban over-predicted during this period. This indicates that this busy road close to AUN contributed about 1/3 of the pollution level to the AUN monitored pollution level over this period (Figure 6.4). These results confirm that major sources near to a receptor can make a considerable contribution to the prediction values.

Figure 6.4 Welford Road and AUN ADMS_Urban NO_2 Predictions

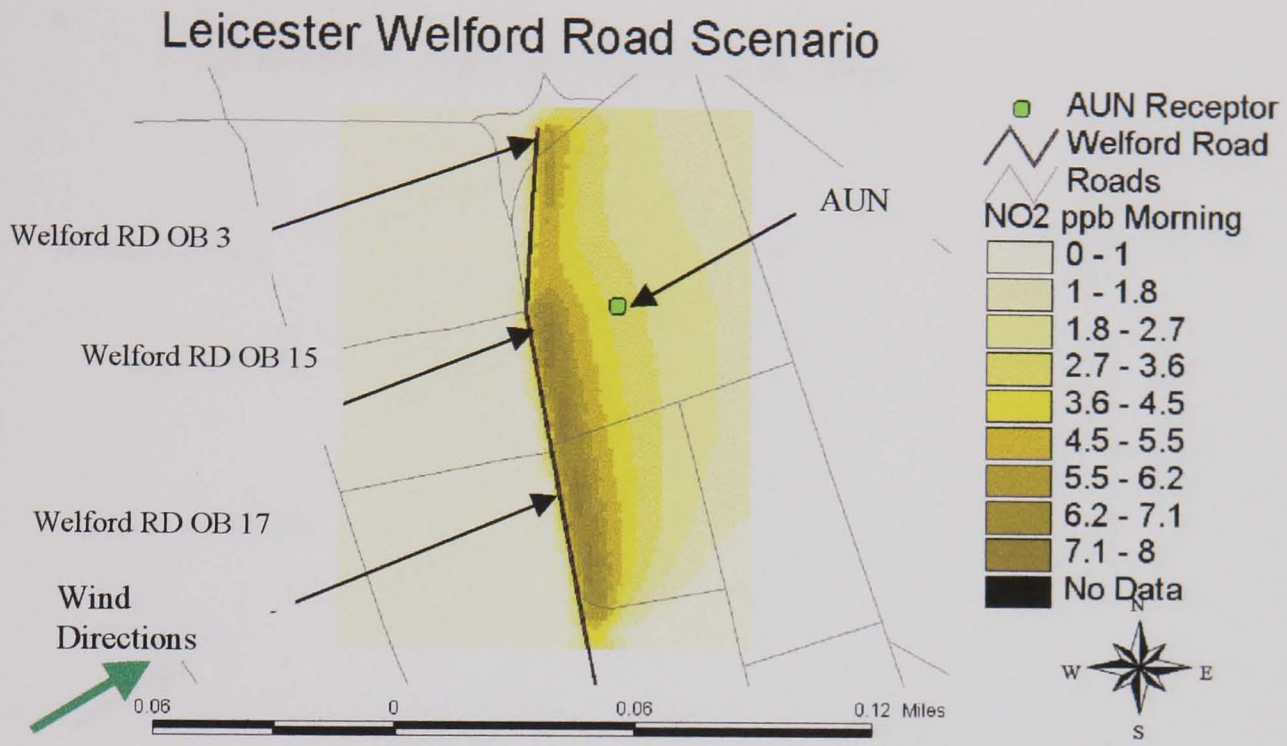


Spatial grid analysis at Welford Road

Three road links, namely Welford Rd OB 3, Welford Rd OB 15 and Welford Rd OB 17, are closest to the AUN site. In order to assess the predicted spatial distribution of pollution along these road links, a "grid output" simulation was undertaken ("grid output" is one of the ADMS_Urban functions to interpret pollution level on a contour plot, using the ArcView GIS software. See section 3.2.3). The meteorological data was from 9th June 1994 to 17th June 1994. During this period, the prevailing wind direction was from the south-west. Figure 6.5 shows the location of Welford Road and these three road links. It should be noted that building turbulence is not modelled in this simulation. Grid output for those three road links also has been plotted (Figure 6.6), It can be seen that near to the road, pollution levels are much higher than those away from road. It is therefore shown ADMS_Urban predictions are sensitive to whether the receptor location is close to road.

Figure 6.5 Welford Road at Leicester

Figure 6.6 Leicester Welford Road Scenario



6.2.3 Effects of Variations to the Emission Database

In order to test the sensitivity of wholesale changes of emission database to the predicted levels, emission rates in the 1996 emissions database were increased 10% and reduced 10%. The receptor used was AUN site, and the meteorological data was from Birmingham Elmdon, 1996.

The impacts of these changes on output values are shown in Tables 6.2-6.5. This shows that if emission rate changes $\pm$10%, the modelled NOx and PM_{10} concentration level change by between about -11.1% and +10.9%, for NO_2 the changes are between -4.1 % and 9.0% levels were derived from non-liner DMC scheme as noted earlier). There appears to be a liner relation for NOx and PM_{10} between the whole set changes in emission database and the predicted levels.

Table 6.2 1996 Emission Database changing 10%

Anunal Average	1996 EDB	1996 EDB +10%		1996 EDB -10%	
		Predicted Values	Relative Changes	Predicted Values	Relative Changes
NO2 (ppb)	24.4	25.5	4.5%	23.1	-5.3%
NOx (ppb)	69.3	76.3	10.1%	62.4	-10.0%
PM_{10} (μg/m3) (non- imported)	7.2	7.9	9.7%	6.4	-11.1%

Table 6.3 NO_2 Concentration at Different Percentile (ppb)

NO_2	1996 EDB	1996 EDB +10%		1996 EDB -10%	
		Predicted Values	Relative Changes	Predicted Values	Relative Changes
99th percentile	51.1	54.1	5.9%	48.6	-4.9%
80th percentile	35.4	36.6	3.4%	34.0	-4.1%
50th percentile	26.4	27.9	5.7%	24.9	-5.7%
30th percentile	16.9	18.1	7.1%	15.6	-7.7%
20th percentile	11.1	12.1	9.0%	10.1	-9.0%

Table 6.4 NO_x Concentration at Different Percentile (ppb)

NOx	1996 EDB	1996 EDB +10%		1996 EDB -10%	
		Predicted Values	Relative Changes	Predicted Values	Relative Changes
99th percentile	364.2	400.6	10.0%	327.8	-10.0%
80th percentile	100.6	110.6	9.9%	90.5	-10.0%
50th percentile	53.5	58.9	9.9%	48.2	-9.9%
30th percentile	27.1	29.8	10.0%	24.4	-10.0%
20th percentile	16.1	17.7	10.0%	14.5	-9.9%

Table 6.5 PM_{10} Concentration at Different Percentile ($\mu g/m^3$)

PM_{10} (non-imported)	1996 EDB	1996 EDB +10%		1996 EDB -10%	
		Predicted Values	Relative Changes	Predicted Values	Relative Changes
99th percentile	34.8	38.3	10.1%	31.3	-10.1%
80th percentile	10.1	11.2	10.9%	9.1	-9.9%
50th percentile	5.7	6.3	10.5%	5.1	-10.5%
30th percentile	3.3	3.6	9.0%	3.0	-9.0%
20th percentile	1.7	1.9	11.7%	1.5	-11.7%

6.3 MODEL PREDICTIONS FOR NON-AUN SITES IN LEICESTER

There are approximately 10 NO_x analysers (measuring NO_2, NO and NOx values, but only NO_2 data are made available) and PM_{10} roadside monitoring sites in Leicester (see Chapter 4, section 4.2). These monitoring sites also provide valuable data resources for the model validation. In order to reveal the performance of ADMS_Urban in predicting the pollution levels at locations other than the AUN site, these monitoring points were chosen as different receptor points for ADMS_Urban scenarios. The details of monitoring data sets can be found at Table 6.7 and their locations are shown in Figure 6.7.

Figure 6.7 Other Receptors at Leicester

Air quality monitors in Leicester can be classified by location type (Table 6.6), i.e. urban background, roadside or kerbside according to their geographic locations and their

surrounding environment. ADMS_Urban modelled values are compared with the monitored values during the period when monitored data are available.

Table 6.6 Monitoring Datasets and Receptor Points for Modelling in Leicester

Reference	Location	Location Classification	Coordinates	Data available
RM1	AUN	Urban Centre	458763 304065	1994 onwards
RM2	LAMS Harrison Road	Urban Centre	460120 306890	14 Feb 1997-15 Feb 1998
RM3	LAMS Narborough Road	Roadside	456575 302128	June 1996-14 Feb 1997
RM4	LAMS Judgemeadow School	Urban Background	463321 303073	15 September 1998-present
RM5	Saffron Lane	Roadside	458543 301937	NO_2, 97, 98, 99
RM6	Bassett Street	Roadside	457788 305444	NO_2, 05/05/97-31/12/97, 98, 99
RM7	Imperial Avenue	Roadside	457245 303040	NO_2, PM_{10}, 13/8/98
RM8	Melton Road	Kerbside	459528 306316	PM_{10} 2/10/98-31/12/98, NO_2 PM_{10},99
RM9	Abbey Lane	Kerbside	458474 306885	NO_2 1/11/98, PM_{10},99
RM10	Soar Valley Way	Roadside	457083 300156	Unknown

6.3.1 Prediction for NO_2 at Four Sites

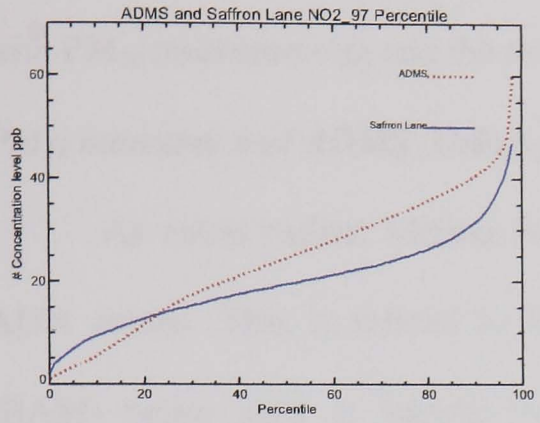
The comparison of the monitored NO_2 level and modelled NO_2 level at different receptors are shown in Table 6.7 and Figure 6.8. It can be seen from Table 6.8, ADMS_Urban under-predicted NO_2 values at Saffron Lane and Bassett Street in 1997 and 1998, but over-predicted NO_2 values at Imperial Avenue and Abbey Lane in 1998.

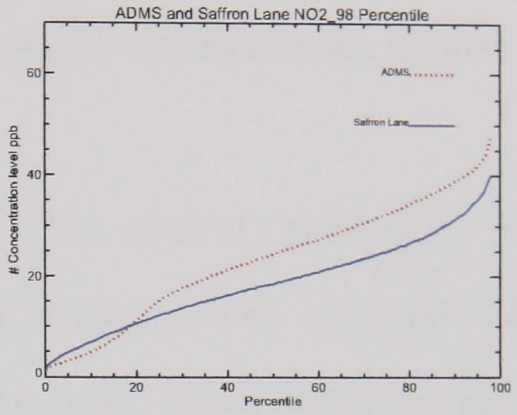
Table 6.7 NO_2 Comparison at Different Receptors

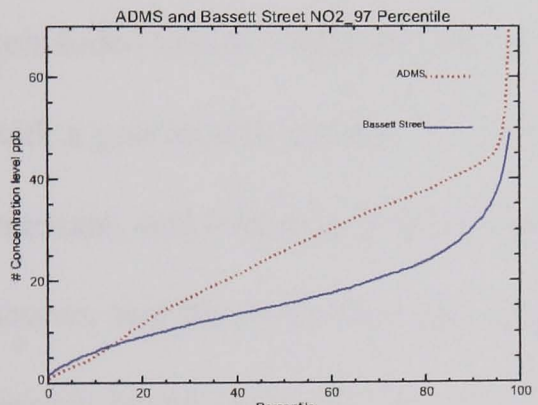
1997	Receptors Location	ADMS_Urban NO_2(ppb)	Monitored NO_2(ppb)	Correlation Coefficient
RM5	Saffron Lane	24.5	19.9	0.34
RM6	Bassett Street	25.8	16.8	0.4
1998				
RM5	Saffron Lane	23.4	18.6	0.53
RM6	Bassett Street	24.1	18.7	0.26
RM7	Imperial Avenue	22.2	27.7	0.28
RM9	Abbey Lane	21.9	25.7	0.37

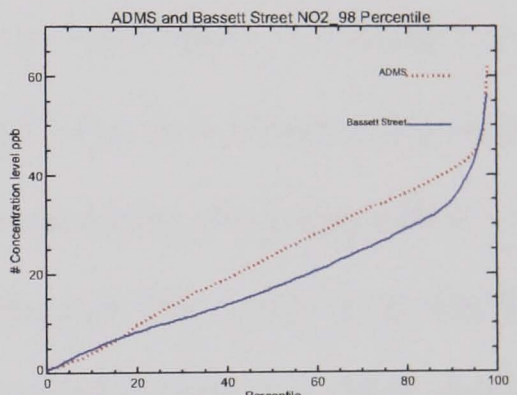
NO_2 modelled value at Saffron Lane in 1997 and 1998 is under-predicted at low percentile (see Figure 6.8), the crossing point is at about 30% percentile, then over-predicted at high percentiles. Figure 6.8 also indicates for NO_2 modelled value at Bassett Street in 1997 and 1998 at low percentile had better agreement, but over predicted when percentile is higher than about 15^{th} percentile. It also shows that for NO_2 at Imperial Avenue in 1998, ADMS_Urban modelled value are constantly under prediction. However, for NO_2 at Abbey Lane in 1998, ADMS_Urban is under predicted when below 75^{th} percentile, but a little over predicted when the percentile is higher than about 75^{th} percentile. Comparing the predicted percentile lines for these receptors (RM5, RM6, RM7 and RM9, Figure 6.8) with the predicted percentile lines for AUN sites (Figure 5.2), the variation in ADMS_Urban predictions for roadside receptors (i.e. Rm6, Bassett Street) are slightly larger than those for urban background receptor (i.e. AUN site).

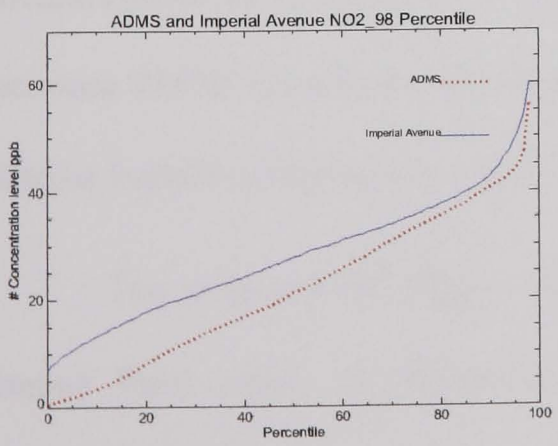
Figure 6.8 ADMS_Urban Output at Various Receptors

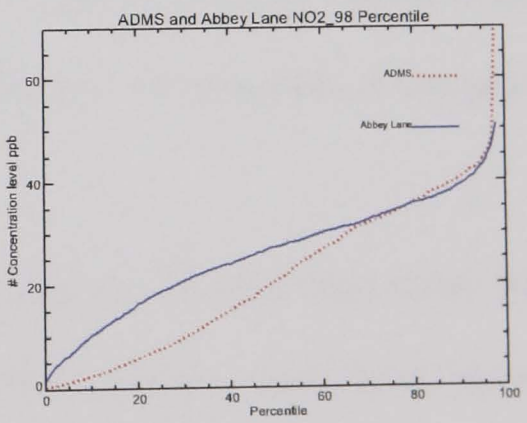












6.3.2 PM_{10} Prediction at Two Sites

Further to the PM_{10} modelling in Chapter 5, roadside PM_{10} predictions comparing with PM_{10} measurements and the street canyon effects, are discussed in this section.

PM_{10} monitors and ADMS_Urban prediction

As noted earlier, Melton Road monitored PM_{10} values are much higher than that AUN values. This is related to the gravimetric instrument Beta Attenuation Monitors (BAM) being used at Melton Road monitoring point. At Imperial Avenue, TEOM instrument is used (details about the analyser can also be found in Chapter 4).

The recently published Airborne Particles Expert Group (APEG, 1999) report concluded that at concentrations around 50 $\mu g/m^3$ the TEOM tends to under-read compared with a gravimetric sampler (i.e. BAM) by between 15 and 30%. However, this effect is not constant, and varies depending upon the mass concentration, the distance from a specific source, and the environmental conditions. Monitoring of PM_{10} levels in the UK has been largely based upon the use of TEOM analysers (APEG, 1999), e.g. AUN stations. The existing objective, which was based upon the air quality standard recommended by the Expert Panel on Air Quality Standards (EPAQS), has been largely based upon measurements made using the TEOM instrument. There is therefore a direct relationship between TEOM measurements and the existing objective (related PM_{10} investigations can also be found in Chapter 5, section 5.4.3).

The proposed EU Stage 1 Limit Values (50$\mu g/m^3$, 24 hour limit value; 40$\mu g/m^3$, annual limit value, as proposed in August 1999), however have been based upon

measurements made using a range of different samplers, and the Directive specifies a gravimetric (i.e. BAM) reference method. There is therefore a potential inconsistency between measurements of PM_{10} concentrations made using a TEOM analyser and the proposed objectives - for example, a daily mean concentration of 45 $\mu g/m^3$ measured using a TEOM analyser could be underestimating the 'gravimetric' concentration by 15 $\mu g/m^3$ or more. So as suggested by APEG report, it is necessary to apply a 'correction factor' when assessing TEOM measured concentrations against the proposed EU objectives. A constant factor of 1.3 has been used in the APEG report, and is applied to all TEOM measured concentrations. For example, a TEOM concentration of 20 $\mu g/m^3$ would be expressed as 20 x 1.3 = 26 $\mu g/m^3$, gravimetric (BAM). To avoid confusion, it is recommended to clearly identify the units of PM_{10} concentrations (AQM, 1999), for example, all data are to be expressed as [$\mu g/m^3$, TEOM] or [$\mu g/m^3$, gravimetric (BAM)] as appropriate.

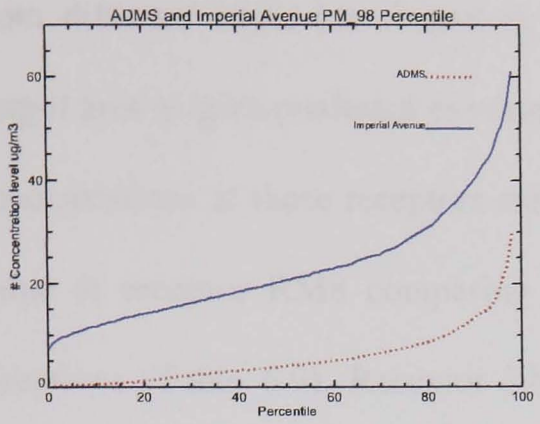
Noting the difference between TEOM and BAM measurements, the average of monitored values and ADMS_Urban predicted values are shown in Table 6.8. The percentile analysis of PM_{10} at Melton road and Imperial Avenue are shown in Figure 6.10. TEOM monitors are installed at Imperial Avenue; BAM monitors are installed at Melton Road.

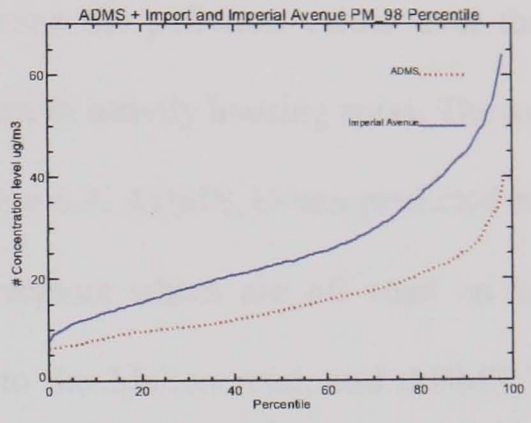
Table 6.8 PM_{10} Predicted Value and Monitored Value at Melton Road and Imperial Avenue Average over Data Available Period 2/10/1998-31/12/1998 ($\mu g/m^3$)

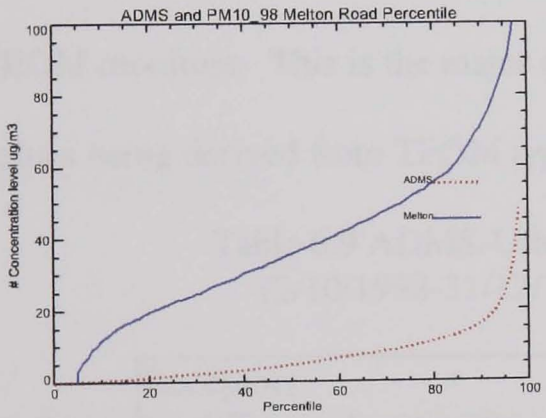
Receptor	Location	ADMS predicted Average	Monitored Average
RM7	Imperial Avenue (TEOM)	5.7	22.9
RM8	Melton Road (BAM)	7.2	40.1
		ADMS Predicted +Imported	Monitored Average
RM7	Imperial Avenue (TEOM)	16.8	22.9
RM8	Melton Road (BAM)	18.3	40.1

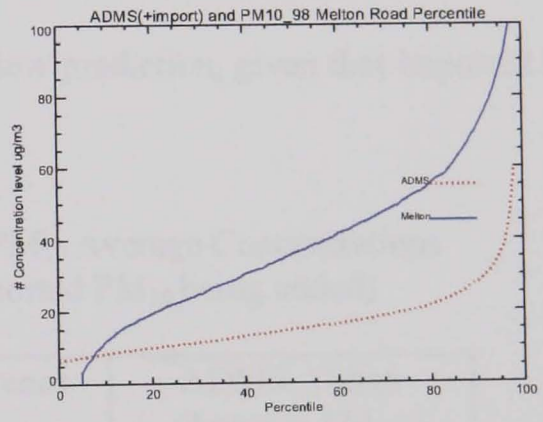
The imported values were derived from remote background sites as annual average $11.1\mu g/m^3$ (the methodology is same as described in Chapter 5, Table 5.10. As the sulphate data at remote sites is currently not available for 1998, the secondary and coarse annual average value here used the data in 1997 instead). It should be noted which monitors have been used when comparing the modelled PM_{10} values with monitored values, as discussed above, there is a significant difference between BAM values and TEOM monitor values. The imported background values were derived from TEOM type monitor. It can be found that BAM monitor on Melton road gave much higher reading than that of TEOM monitor on Imperial Avenue (Table 6.8). ADMS_Urban model gives lower predicted average values at both busy road sites, particularly, comparing with BAM monitor at Melton Road.

Figure 6.9 ADMS_Urban PM_{10} Melton Road and Imperial Avenue







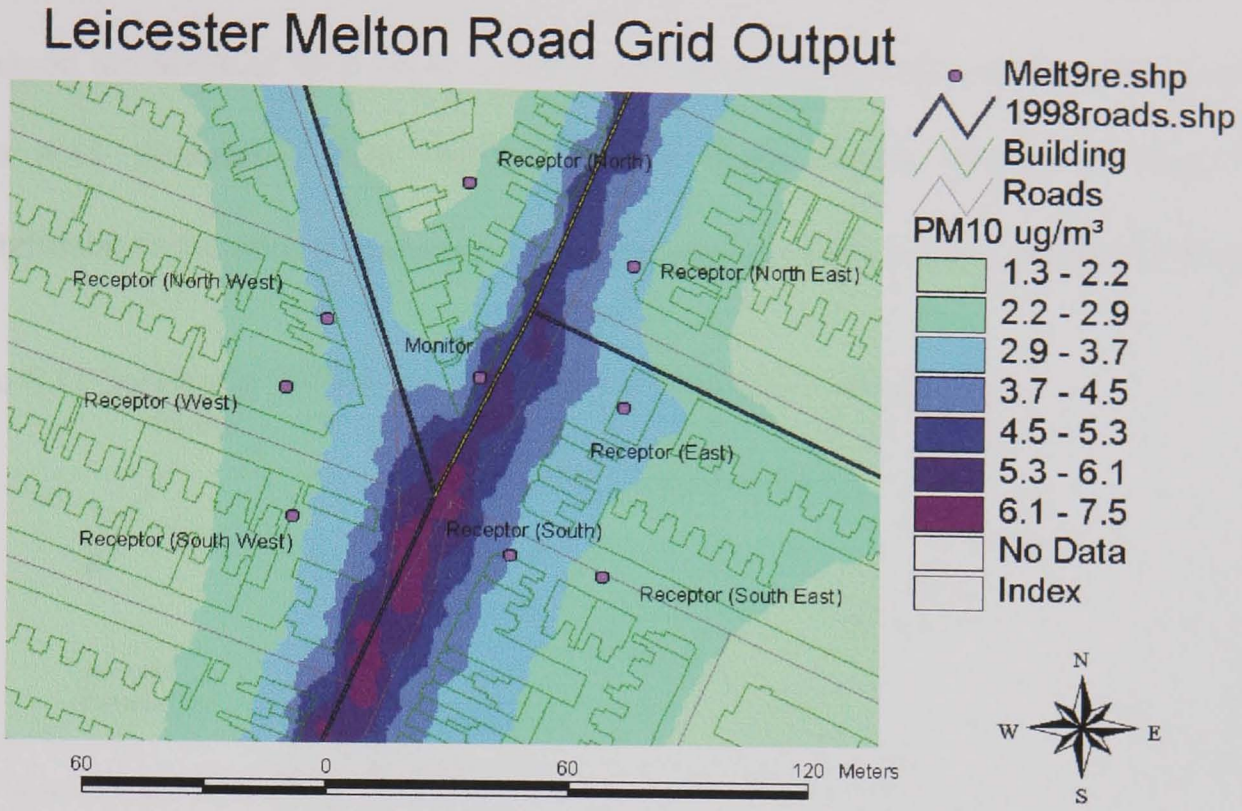


It is shown clearly on the grid output over this area that the areas near to roads have higher concentration values than that far away from roads (Figure 6.10). Eight receptors from different angle are chosen in order to illustrate the pollution values over the grid output area to give predicted environmental exposure in heavily housing areas. The average concentrations at these receptors are shown in Table 6.9. ADMS_Urban predicted highest value at receptor RM8 comparing with other receptors which are off road on various directions (Table 6.9). Receptor RM8 is closest to the Melton road, and ADMS_Urban predicted values are higher than that of other receptors. PM_{10} levels were under predicted more at Melton road than that of at Imperial Avenue, even when imported PM_{10} values were added (Figure 6.9). It is noted that BAM instrument was used at Melton Road. As discussed in this section, BAM instrument would give up to 30% higher reading than that of TEOM monitors. This is the major cause of such low prediction, given that imported PM_{10} values being derived from TEOM type monitors.

Table 6.9 ADMS-Urban Predicted PM_{10} Average Concentrations (2/10/1998-31/12/1998) (No imported PM_{10} being added)

Receptors (at different directions)	Reference	ADMS_Urban Average PM_{10} (μg/m3)
Receptor Melton Road Monitor	RM8	7.2
Receptor (North)	Rnorth	4.4
Receptor (West)	Rwest	3.5
Receptor (East)	Reast	4.5
Receptor (South)	Rsouth	4.8
Receptor (North East)	Rne	5.3
Receptor (North West)	Rnw	3.8
Receptor (South West)	Rsw	3.9
Receptor (South East)	Rse	3.9

Figure 6.10 Leicester Melton Road Grid Output



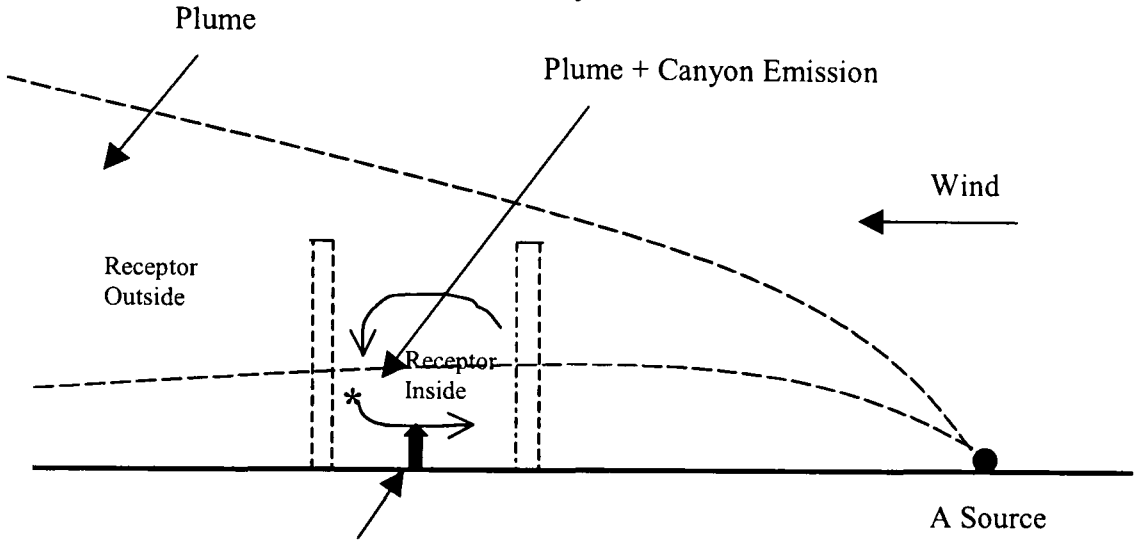
Street canyon effects

There are considerable residential and commercial buildings along Melton Road, these form a street canyon. In order to test street canyon module in ADMS_Urban and whether it would provide a better prediction for this type of situation, following are discussed.

The street canyon model in ADMS_Urban predicts concentrations at the points on a road bordered by high buildings (>2m), and is integrated with the prediction of concentrations at off-road points. It is used for calculating the concentration at points which lie in the roads lined with buildings with heights greater than 2m. Concentrations inside the

road tend to the non-canyon results in the limits as the canyon height is reduced to zero or the road width increased to over twice the canyon height. Concentrations at points outside the canyon are identical with those which would be obtained if the road were not a canyon. Figure 6.11 illustrates while wind crosses a street canyon when the wind blows perpendicular to the axis of the street (across the street) a re-circulating region is set up.

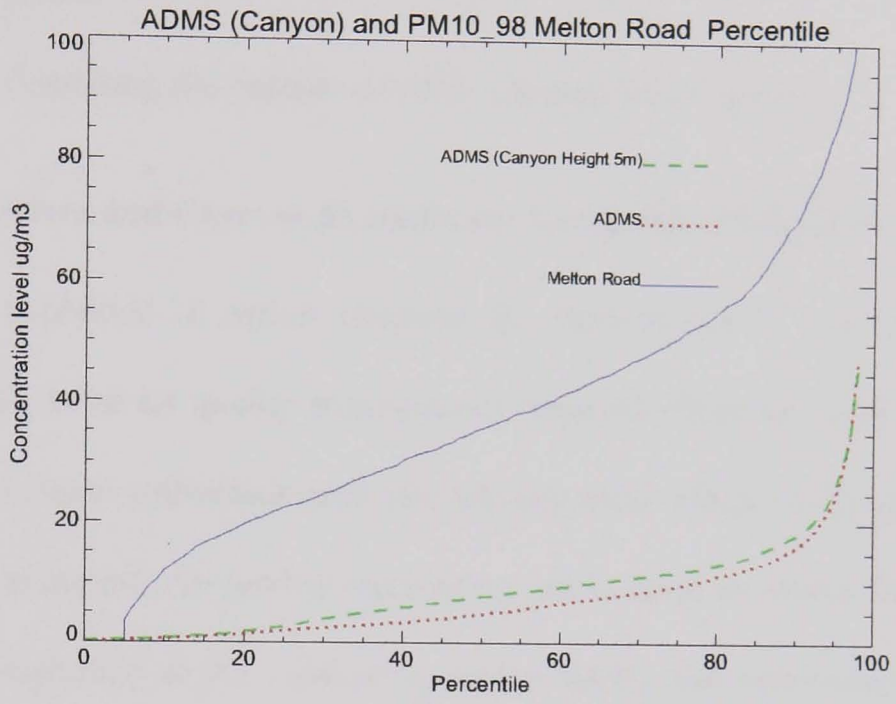
Figure 6.11 Schematic Illustration of Canyon Influence to a Plume



In general model scenarios, street canyon effects are not considered in this study as no data are apparently available. For the purpose of testing this effect, the canyon height 5m is added. Meteorological data used was from 2nd October to 31st December 1998, Leicester. With canyon height, the average of modelled Melton Road PM_{10} value was increased from 7.2 $\mu g/m^3$ to 8.9 $\mu g/m^3$ (no imported values being added).

The percentile plot of this change can be found in Figure 6.12. This demonstrates the canyon effects to the model output. While modelling a receptor near to a road, i.e. Melton Road, it should be noted that street canyon height (if > 2m) needs to be specified, as this will affect the predictions.

Figure 6.12 ADMS (Canyon) and PM_{10}_98 Melton Road Percentile
(No imported values being added)



6.4 STRATEGIC MODELLING

Previous sections of this study have focussed on the performance of ADMS_Urban to predict pollution concentrations at given locations. Model predictions were compared with monitored data. This section demonstrates the use of ADMS_Urban for strategic modelling of air quality. Generally, this involves some form of scenario testing whereby model input factors are changed and the impact on predicted air quality can be assessed. For 2005, the projected vehicle emission factors are generally lower than that of present time.

This study has been based on the application of ADMS_Urban in Leicester, and this chapter will therefore consider some of the principal strategic modelling tasks that the model could be used for in the City, namely:

- Predicting current and future air quality based on projected changes in emission levels
- Assessing the impact of traffic schemes on air quality

6.4.1 Objectives and Current Exceedences for the Key Pollutants

As explained in earlier chapters, the introduction of the Environment Act 1995 imposed new local air quality management responsibilities on local authorities in the UK. In particular, local authorities must identify any areas where air quality objectives for 2005 will not be achieved. Air quality monitoring can be used as a basis for assessing current air quality (though only at the monitoring station itself), but cannot be readily used to assess future levels of air pollution. It is for strategic tasks such as this that air quality models have an important role.

Previous chapters have discussed the nature of air pollution problems in Leicester, and have highlighted nitrogen dioxide NO_2 and PM_{10} as two of the pollutants of primary concern. The National Air Quality Strategy (DoE, 1999) also identifies these as perhaps the two pollutants of most widespread concern. Therefore whilst the Review and Assessment (DoE, 1999) process involves 6 prescribed pollutants, this section will concentrate on NO_2 and PM_{10} alone.

The Objective for Nitrogen Dioxide and the Exceedences

There are two Objectives for nitrogen dioxide: An hourly mean of 150 ppb or less and an annual mean of 21ppb or less (HM Government, 1998b). The annual Objective can clearly be deemed to be breached at any location where persons are reasonably likely to be exposed non-occupationally near ground level over the averaging period, e.g. areas of housing. Since the main source of nitrogen dioxide in Leicester is motor traffic, concentrations will tend to be highest near to very busy or highly congested roads.

As reported by LCC (1999), Sixty-four road links were identified in Leicester which had annual average daily traffic flows greater than 20,000 vehicles which is considered as large contributors to air pollution. In addition, around twelve road links were identified outside the boundaries of the City but in sufficiently close proximity to exert a significant influence. No current or prospective industrial source was identified as being a significant contributor to air pollution, according to the criteria set in Guidance Note LAQM. TG4 (98) (DETR, 1997h).

The ratified annual mean concentrations for Nitrogen dioxide (Table 6.10) for the site are as follows:

Table 6.10 NO_2 AUN Annual Mean in Leicester

Year	Annual Mean (ppb)
1994	23
1995	23
1996	22
1997	21

It can be seen that, while the air quality Objective expressed as an annual mean is exceeded for all of the years 1994 to 1996, the current national criterion of 30 ppb is not exceeded in any year.

Leicester re-locatable air monitoring station (LAMS) was located at Rushey Mead Primary School from March 1997 to February 1998. Over this period, the annual mean for nitrogen dioxide was 15.3 ppb. (The Objective for 2005 is 21 ppb).

The Objective for PM_{10} and the Exceedences

The Objective for PM_{10} is 50 $\mu g/m^3$ when expressed as the 99th percentile of daily maximum running 24-hour means. This means that the highest values for the twenty-four 24-hour running means in each day in any given calendar year are taken. The 99th percentile of those 365 values (366 in a leap year) is calculated, rounded to the nearest whole day. The effect of this is that the value of 50 $\mu g/m^3$ for the daily maximum running 24-hour means can be exceeded for 4 days any year before the statutory Objective is deemed to have been breached for that year (HM Government, 1998b).

However, this is likely to be superseded by the criteria now adopted in the EC Air Quality Daughter Directive (AQDD), Stage 1. This sets two permissible levels:

- A maximum annual mean of 40 $\mu g.m^{-3}$.
- A maximum 24-hour mean of 50 $\mu g.m^{-3}$, with up to 35 exceedences allowed per year (approximating to the 90th percentile).

In addition, as cited from the recent analysis of the nature and origins different fractions of airborne particles by the Airborne Particles Expert Group (APEG, 1999):

- The understanding that a substantial proportion of prevalent levels of particulates are of remote origin and not therefore susceptible to local control, for example by traffic management measures;
- The consequent appreciation that the existing Objective is unrealistic.

The DETR has also provisionally advised (DETR, 1999):

- Where there is the possibility that the Air Quality Daughter Directive (AQDD) Stage 1 standard will be breached, to proceed, using that standard as a baseline.
- Where the AQDD standard does not appear at risk of being breached, to await further guidance.

Significant Sources of PM_{10} in Leicester

As noted earlier, sixty-four road sources are identified as significant contributors to the air pollution in Leicester. Five "Part A" processes identified by the Leicester City Council as having the potential to be significant emitters of PM_{10}, however the emission data for PM_{10} are not available. No "Part B" processes were identified as significant emitters. In a survey carried out by the Leicester City Council, there are no known proposals to establish further processes in or around Leicester which will emit significant quantities of PM_{10}. Industrial processes with uncontrolled/fugitive emissions of significant PM_{10} were not found. The statutory Air Quality Objective for PM_{10} breached at AUN site from year 1994 to 1997 was summarised in Table 6.12.

Table 6.11 PM_{10} 99th percentile of maximum daily 24-hour running average ($\mu g/m^3$)

Year	99th percentile of maximum daily 24-hour running average PM_{10} concentrations (TEOM, $\mu g/m^3$) (Objective = 50 $\mu g/m^3$)
1994	61
1995	52
1996	75
1997	58

As noted earlier, Leicester re-locatable air monitoring station (LAMS) was located at Rushey Mead Primary School, Harrison Road, from March 1997 to February 1998. Over this period, the Objective value of 50 $\mu g.m^{-3}$ was exceeded on 12 days; i.e. applying the 99th percentile, the Air Quality Objective was breached on 8 days in 1997 and 4 days in 1998. Exceeding values were as shown in Table 6.12.

Table 6.12 PM_{10} exceedence values at LAMS (December 1997 to February 1998)

Date	Maximum daily 24-hour running average PM_{10} concentrations (TEOM, $\mu g/m^3$). (Objective = 50 $\mu g/m^3$)
12/08/97	52
13/08/97	52
21/08/97	53
22/08/97	59
31/10/97	57
01/11/97	80
02/11/97	87
03/11/97	55
29/01/98	60
30/01/98	68
31/01/98	76
01/02/98	76

It should be noted that both winter and summer exceedences occurred and also LAMS is a "semi-background" site and that locations which meet the exposure criteria exist in closer proximity to nearby heavily-trafficked roads. As PM_{10} has had considerable exceedence records over the years, it becomes one of the major concerns of air pollution control in Leicester.

6.4.2 Leicester Emissions For 2005

The reductions necessary to achieve the air quality objectives by 2005, for most or all of the defined key pollutants, will come from the national measures. However, additional local action may also be necessary. In the majority of urban areas, road traffic pollution will be the principal source of air quality problems. Therefore, in developing action plans for Air Quality Management Areas, the contribution which local traffic makes to pollutant levels in their area and, whether local traffic management can play a part in making improvements will need to be considered.

The basic TRIPS Model output was used as line-source (traffic) input data for the ADMS_Urban model (Chapter 4, Section 4.2.3). However, it was noted that the TRIPS model output needed updating prior to its use in dispersion modelling. For example, the existing TRIPS Model outputs were dated from 1995; validation using a programme of actual traffic counts had last been performed in 1996. The traffic base-line used for future atmospheric dispersion modelling was therefore in need of update.

A review and update of the TRIPS Model data was undertaken by LCC. Completed in March 1999 (LCC, 1999), this comprised the following deliverables: output files

compatible with the dispersion model, showing AM and PM peak flows for the road links modelled by the Greater Leicester Traffic Model (GLTM) for 1998 and 2005. These data are also capable of estimating of 24-hour flows for the relevant links. The existing GLTM output was updated to the 1998 standard. This involved updating the highway network within the Model to include highway network changes which had occurred in the intervening period, for example capacity changes, space reduction and reallocation, traffic calming, pedestrianisation, one-way schemes, traffic bans and parking restrictions.

In updating the TRIPS Model data, the levels of traffic growth in 2005 were also projected. The traffic growth figures used for forecasting pollution levels in 2005 were derived from the Leicester City Council's work under the Road Traffic Reduction Act 1997. These data have been used for constructing emission database in 2005 for Leicester.

The Central Leicestershire Strategic Transport Studies (CALTRANS) study set the baseline for future forecasts in 1995. Since then, traffic has grown by an average of about 1% to 2% each year over the whole network (LCC, 1999). Monitoring has shown that road traffic across the central area has reduced in the last three years. In 1997, traffic levels on the Leicester Central Ring Road remained static (actually showing a very small fall). However, growth on the motorway and trunk road network outside the urban area has increased each year by about 3% to 5% (LCC, 1999).

Overall traffic growth was factored into the study in Leicester using data from the National Trip-End Model (NTEM) forecast to project the 1998 patterns of movement to 2005. The overall growth of traffic for the GLTM study area was equal to the 8.8% for the Leicestershire area (LCC, 1999). The results are as in Table 6.13.

Table 6.13 Traffic Growth in 2005 (Data Source: LCC, 1999)
(Vehicle numbers)

AM 1998 Total	102,657
AM 2005 Total	111,651
Growth	8.8%
PM 1998 Total	109,215
PM 2005 Total	118,826
Growth	8.8%

For dispersion modelling purposes, the annual Average Daily Traffic (AADT) is the required input and it was therefore necessary to derive these from the average peak flows generated by the GLTM. This was done by factoring the peak flows by 10 in Leicester's 2005 emission database (LCC, 1999), i.e. it was assumed that the peak represents an average of 10% of daily flow. In practice, the peak to daily flow ratio is observed to vary between sites, areas (urban/rural) and time periods (AM/PM) over a range of about 6% to 11% but a mean ratio of around 10% was considered to be a reasonable approximation over the study area. Speeds within the GLTM are not based on actual traffic speeds but just based on the speed-limits applied to the road links concerned, which is not satisfactory for dispersion modelling purposes as noted earlier. Before inputting vehicle speed to the dispersion model, this was therefore refined by inspecting individual links and amending the speed inputs where appropriate, according to available observations.

It should be noted that the traffic model used has significant limitations. For example: the GLTM is a simple, link-based model and cannot represent traffic behaviour at junctions. The model is only as good as its underlying assumptions e.g. those made about differential growth factors applicable to different regions of the network to represent the impact of future policies and network changes. The GLTM model does not represent every

road on the network and its outputs can only be regarded as indicative for broad, strategic purposes.

The emission database for 2005 was constructed taking the above mentioned factors into account. The strategic modelling using the 2005 emission database is described in the next section.

6.4.3 Projected Change in Vehicle Emission Factors 1995 to 2005

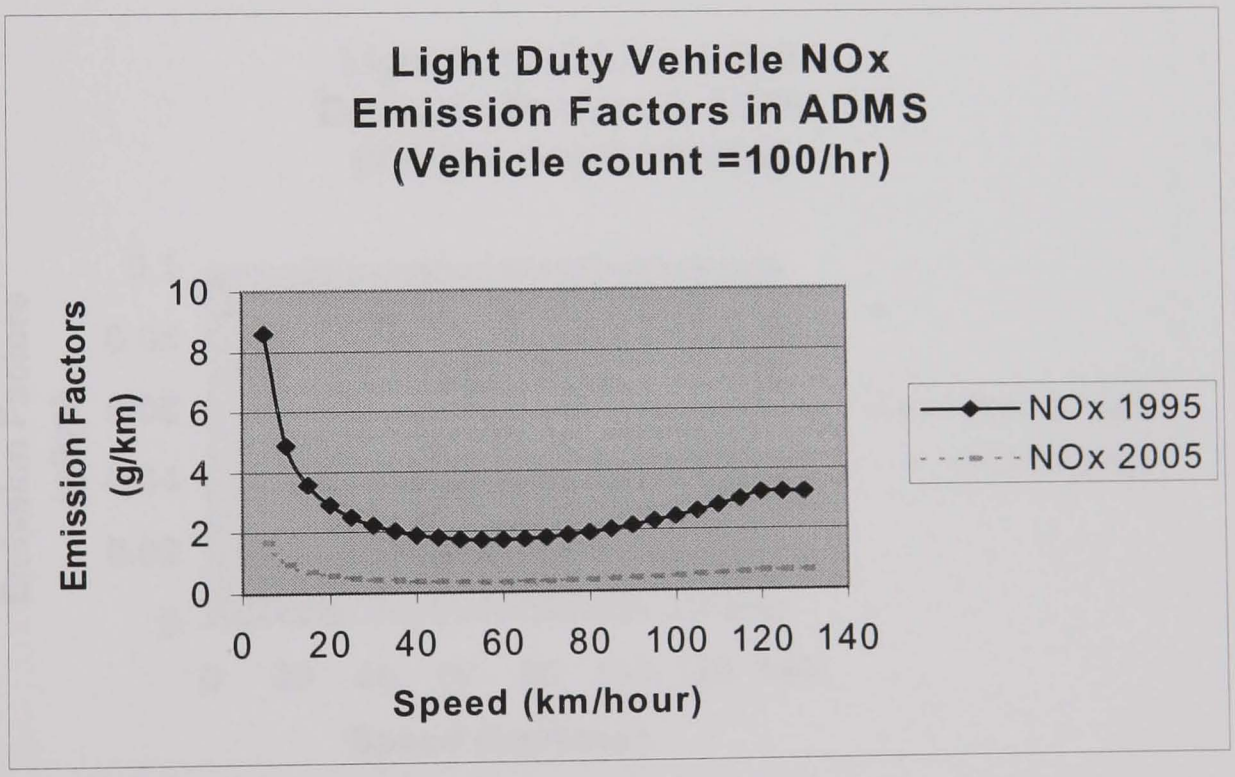
It was considered that different parts of the modelled area of Leicester would experience widely different rates of traffic growth, ranging from substantially positive to somewhat negative. This was based on the various projected impacts of development proposals and traffic schemes in different areas, superimposed upon the generalised projections of UK national traffic forecasts.

Despite significant traffic growth, progressively tighter EU vehicle emissions standards have led to emissions of all local air pollutants being significantly lower than they were ten years ago (DETR, 1999). Further improvements are also expected from the introduction of more stringent EU emissions standards in 2000 and 2005 for new vehicles and the increased number of vehicles in the UK fleet meeting earlier EU emissions standards. For example between 1995 and 2010 NOx emissions are expected to be reduced by around 62% and PM_{10} by 57% (DETR, 1999).

Although general levels of traffic are expected to grow by 2005, new clean fuel technologies will have a more dramatic effect reducing the total emission. These changes are reflected in the emissions factors that are available for model input. Figures 6.13 -6.20

show the vehicle emission factors used in ADMS_Urban for 1995 and 2005 which based on values provided by DMRB. The DMRB emission factors are for driving cycles with the given average speed. A significant drop in emission factors for 2005 can be seen for all pollutants and for all vehicles, though PM_{10} emission factors from light duty vehicle have not been predicted a great decrease (Figure 6.16). Based on these changes, the future air quality for 2005 is likely to be better than at present despite the traffic growth. It is worth noting that in ADMS_Urban, the traffic emission factors are derived from average vehicle speed only. Recent work has shown that emission factors based on real-world drive cycles (i.e. accounting for acceleration, deceleration etc.) can vary greatly from the average speed emission factors[1].

Figure 6.13



[1] Private communication with K. Turpin, IESD, De Montfort University.

Figure 6.14

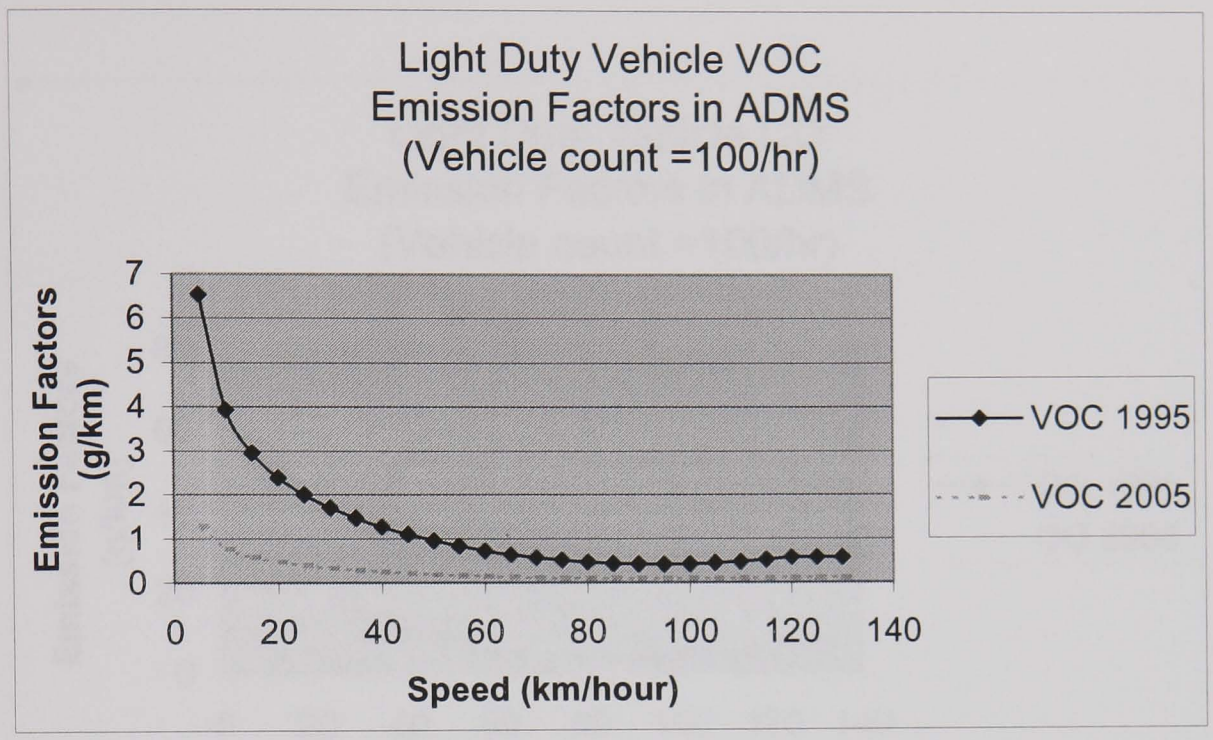


Figure 6.15

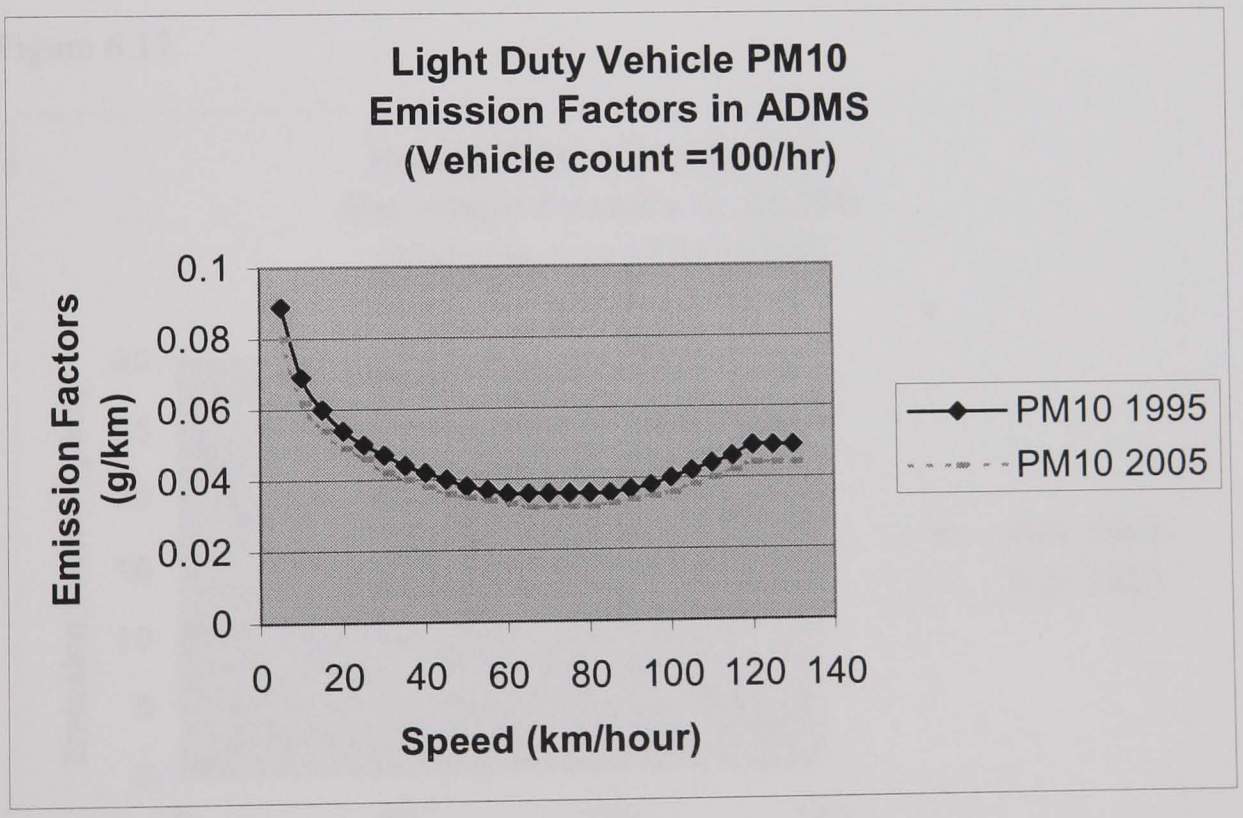


Figure 6.16

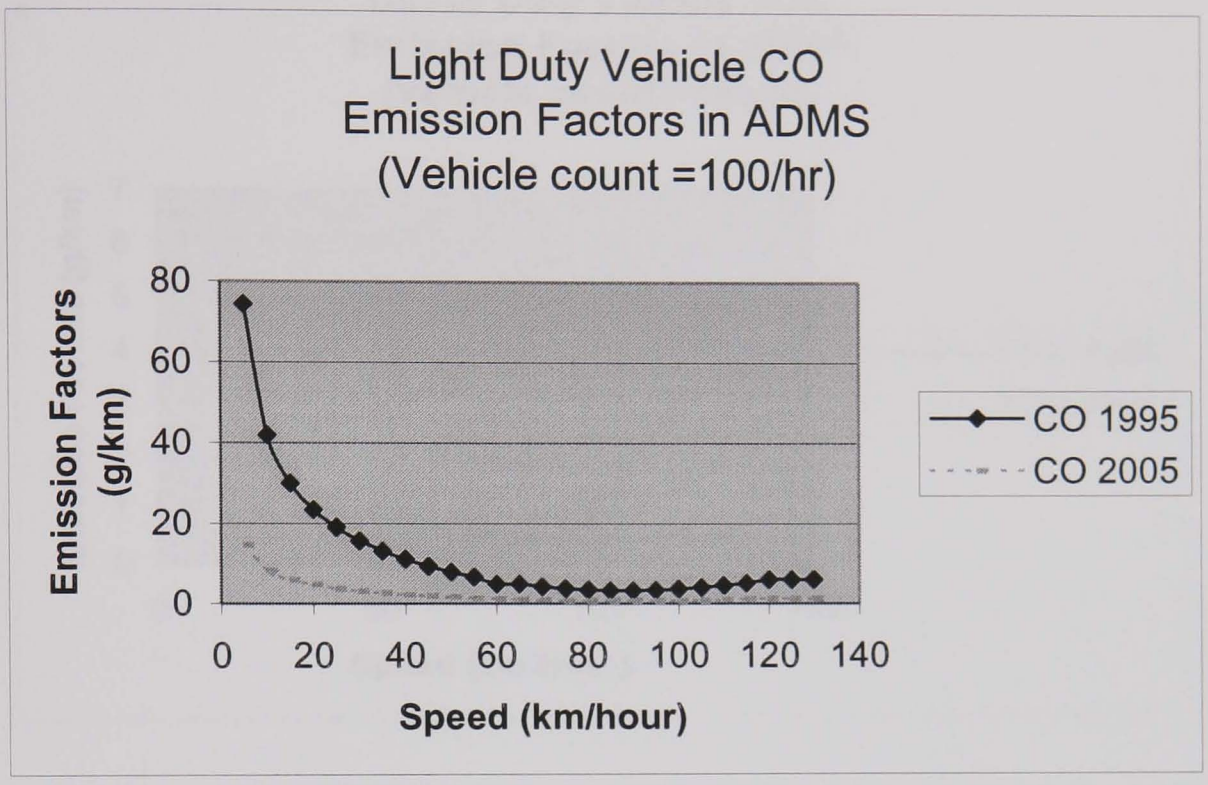


Figure 6.17

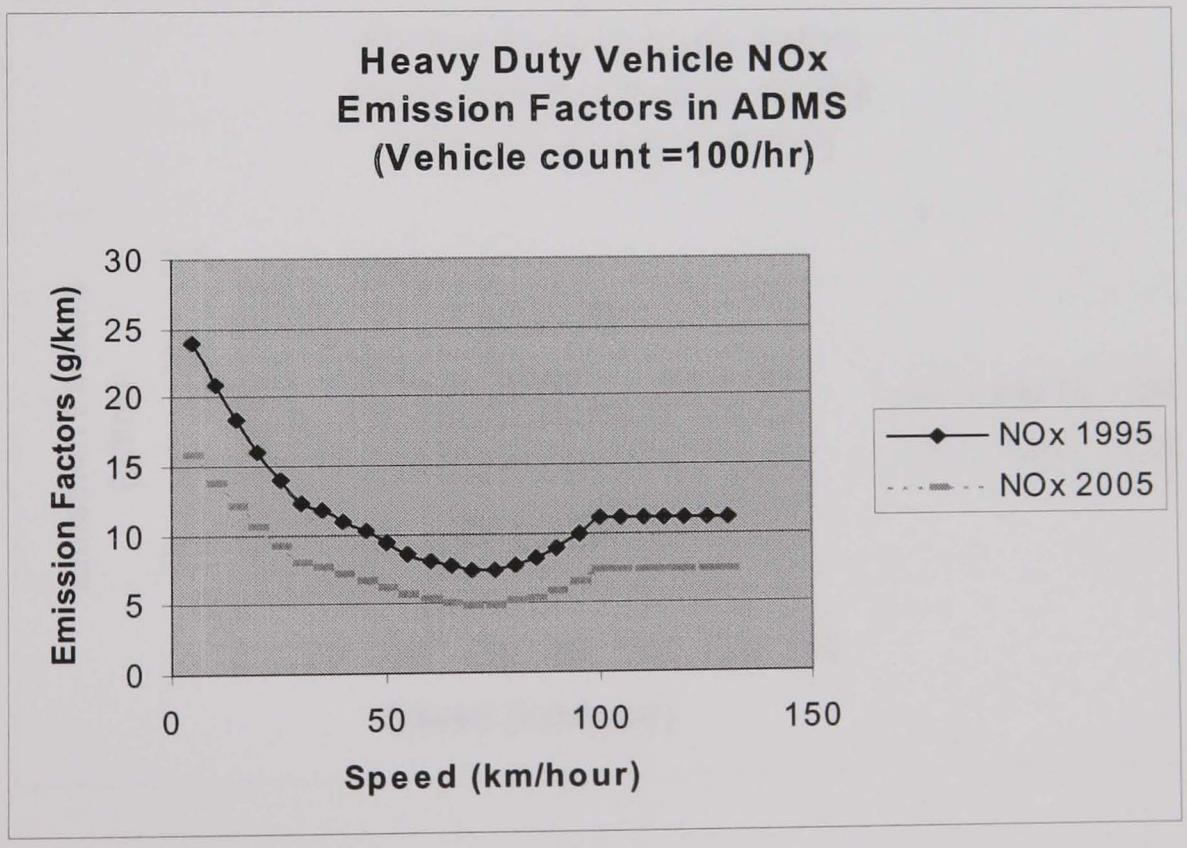


Figure 6.18

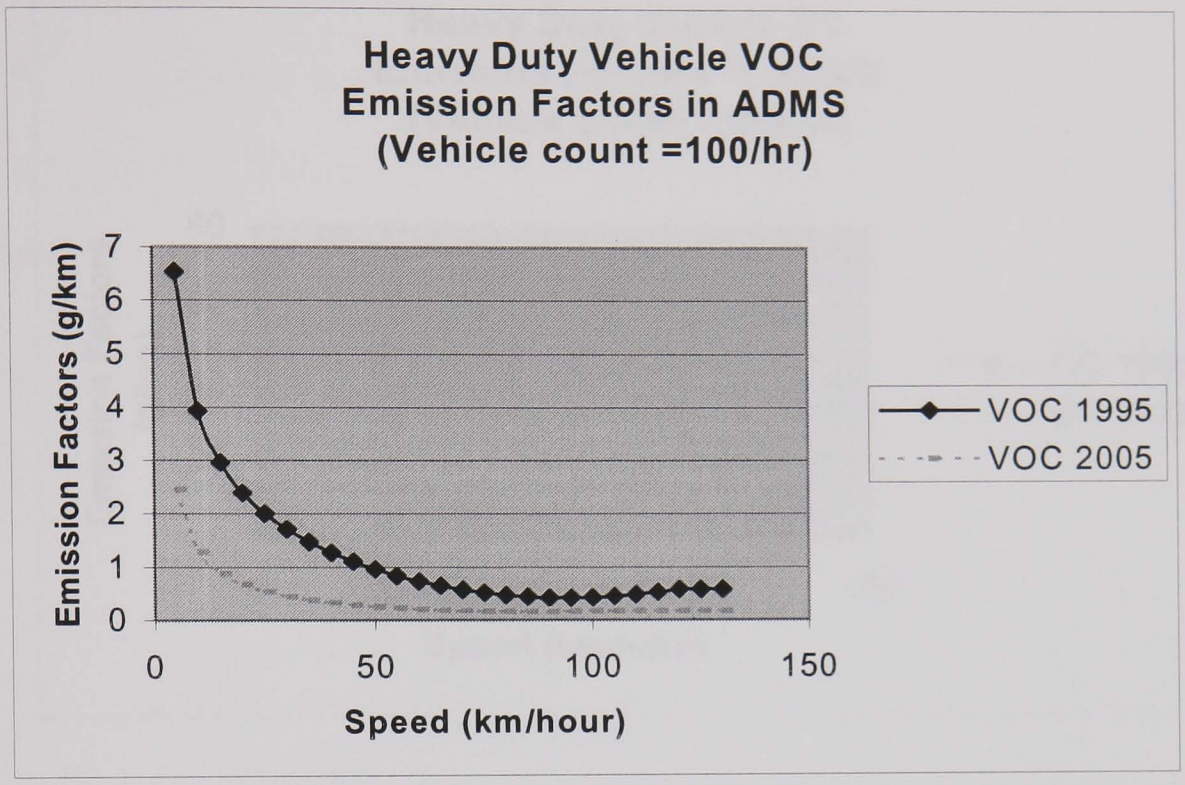


Figure 6.19

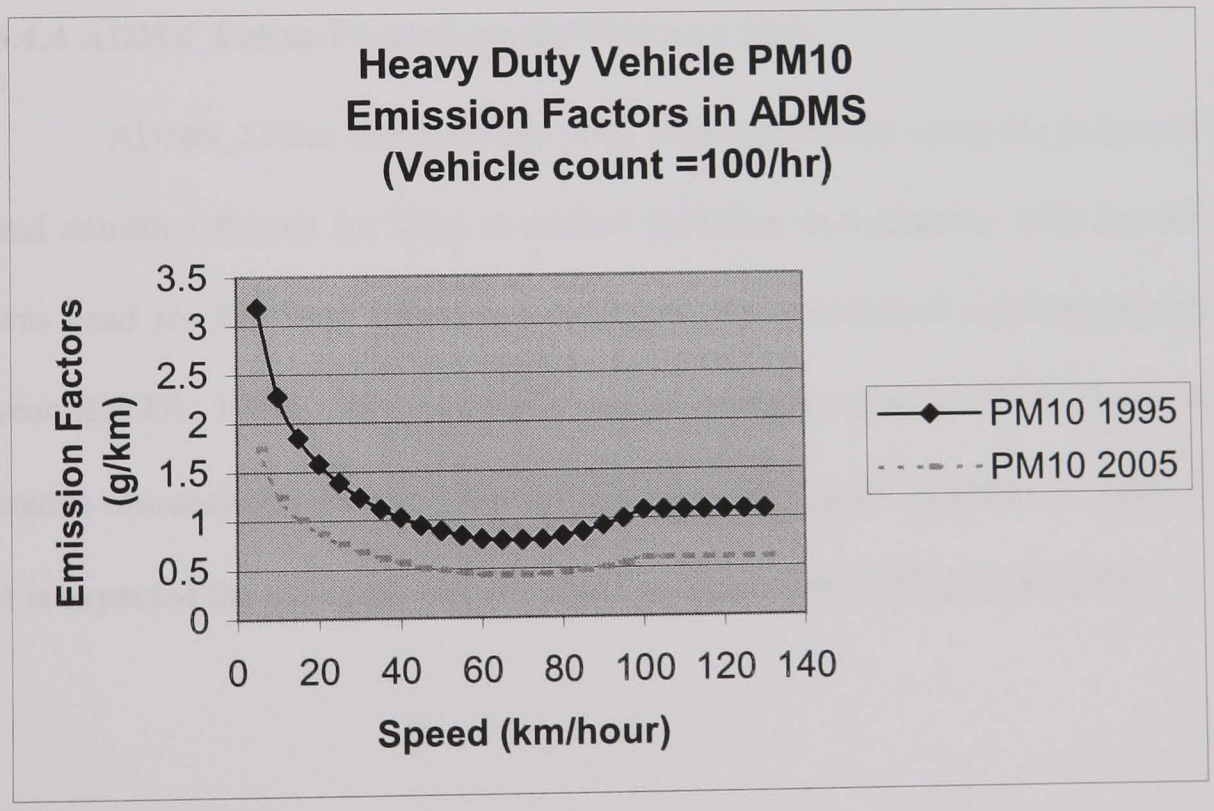
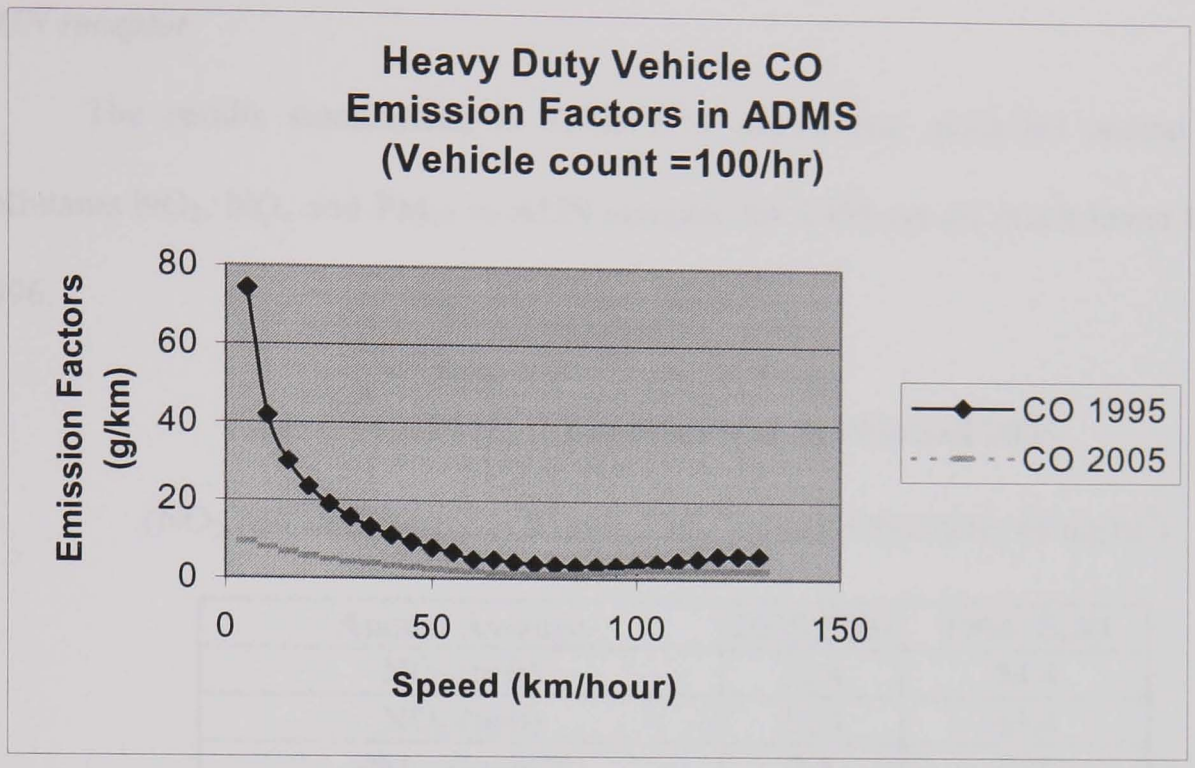


Figure 6.20



6.4.4 ADMS_Urban Predictions for 1996 and 2005

ADMS_Urban scenarios for 2005 were carried out using the projected traffic flows and emission factors for 2005 to predict pollution exceedences. 1996 meteorological data was used for the 2005 scenario as this year was recognised representing typical weather year (DETR, 1999). Imported PM_{10} annual average value for 2005 (from secondary and coarse sources) was used as same as for 1996 (13.3 $\mu g/m^3$, Chapter 5, Table 5.10). Though it is expected the imported values should be reduced in 2005 (DETR, 1999).

AUN receptor

The results summarised in Table 6.14 shows that modelled annual average of pollutants NO_2, NO_x and PM_{10} in AUN receptor for 2005 are all much lower than that for 1996.

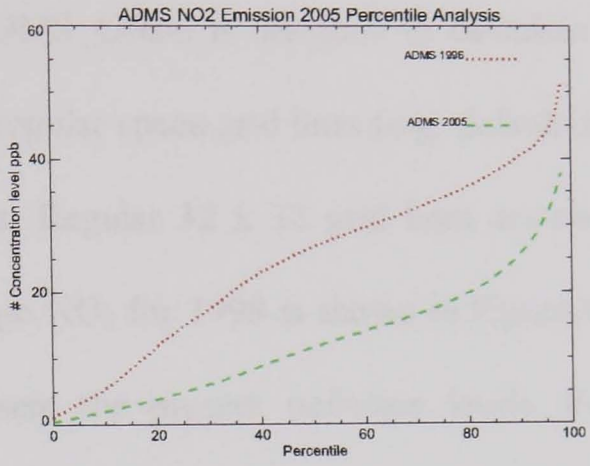
Table 6.14 ADMS_Urban Prediction in 1996 and 2005

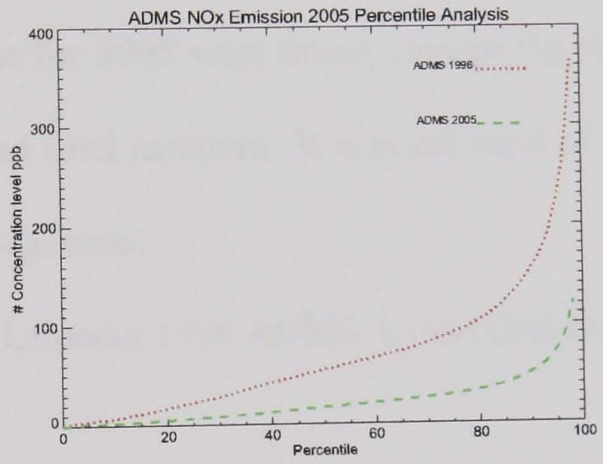
(NO_2 Annual Objective: 21ppb, PM_{10} Annual Objective: 40 $\mu g/m^3$)

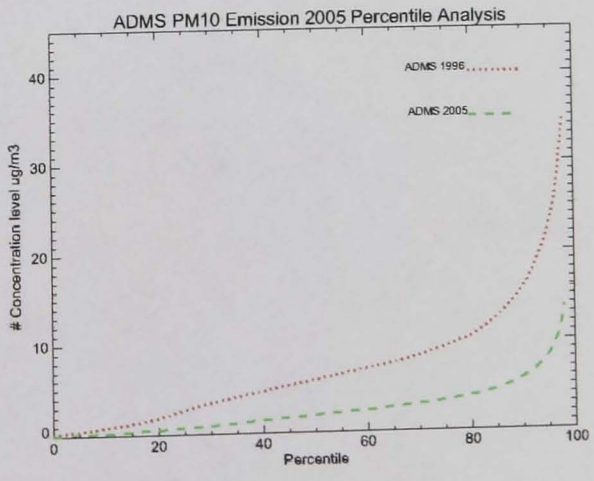
Annual Average	2005 EDB	1996 EDB
NO_2 (ppb)	12.4	24.4
NO_x (ppb)	22.4	69.4
PM_{10} ($\mu g/m^3$)	2.5	7.2
PM_{10}($\mu g/m^3$)+Imported (TEOM)	15.8	20.5

The percentile comparison of the ADMS_Urban predictions for 2005 and 1996 are shown as percentile plots in Figure 6.21. ADMS_Urban predicted values in 2005 are much lower than the predicted values in 1996, especially for the high percentiles, e.g. the predictions for NOx. As only one receptor point may not represent the overall pollution levels, the spatial predictions for 2005 over Leicester area are presented next.

Figure 6.21 ADMS_Urban Prediction in 1996 and 2005 Percentile Analysis



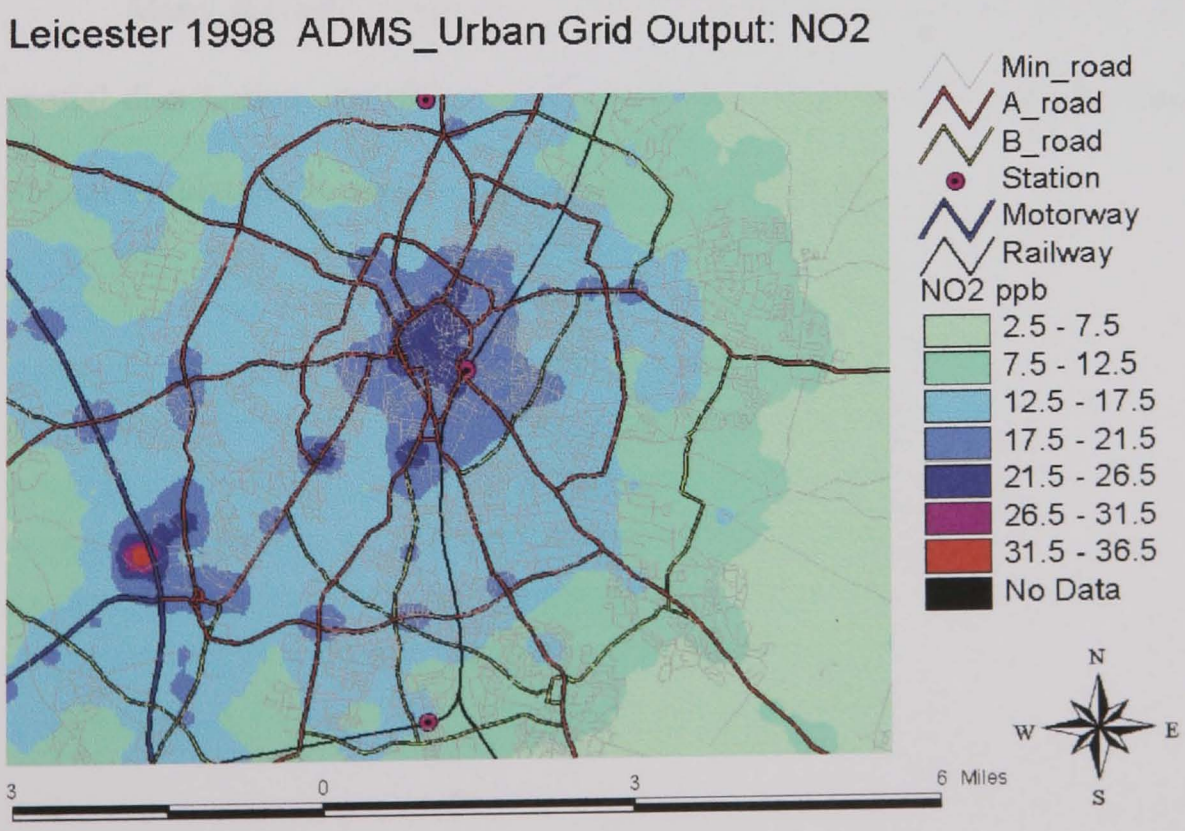




Spatial predictions

A single receptor may not be representative of the air quality over an urban area. "Grid output" in ADMS_Urban is designed to calculate the pollution levels over an area. Cartesian grid with regular space grid lines (e.g. default 32 grid lines) can be chosen for the selected output area. Regular 32 x 32 grid lines are used here. The spatial prediction of annual hourly average NO_2 for 1998 is shown in Figure 6.22. This was the most recent full year data to represent the present pollution levels. For 1998 predictions, some areas, particularly busy roads in the city centre, have exceeded the 2005 objective. Spatial prediction of annual hourly average NO_2 for 2005 is shown in Figure 6.23. However, no areas of exceedences for 2005 were found, though the high pollution levels were predicted at the city centre and road junctions. It is noted most of high values are around city centre area or major road junctions.

Figure 6.22 Leicester 1998 ADMS_Urban Grid Output: NO_2



The "blobs" (Figure 6.23) can occur when a receptor point of regular coincides with a road. "Blobs" are mostly associated with major road sources (or point sources), i.e. a blob at upper left corner on Figure 6.23. This "blob" corresponds to a stretch of the A46 Leicester Western Bypass (dotted line on the map) and also due to other small roads that join or go under the A46 Leicester Western Bypass at that point. A46 Leicester Western Bypass is a new major road between M1 and A46 which is included in the emission database for 2005 but not shown on the current OS map (based on 1996).

An illustration of these regular grid points and main road sources for 2005 can be seen in Figure 6.24. Some road links shown are broken as they are separated from rest of the aggregated small road sources. The road network for 2005 contains more roads (Figure 6.24) than were shown on the OS map (Figure 6.23). It can be seen that "blobs" occur mostly when receptors are superposed on the road sources. Accordingly, spatial plots need to be interpreted with caution.

Many receptor points (i.e. 32 x 32) have to be used to obtain prediction for the spatial distribution of pollutants. This can be computationally very demanding, i.e. for the annual simulation, it can take about a week to complete.

Figure 6.23 Leicester 2005 ADMS_Urban Grid Output: NO_2

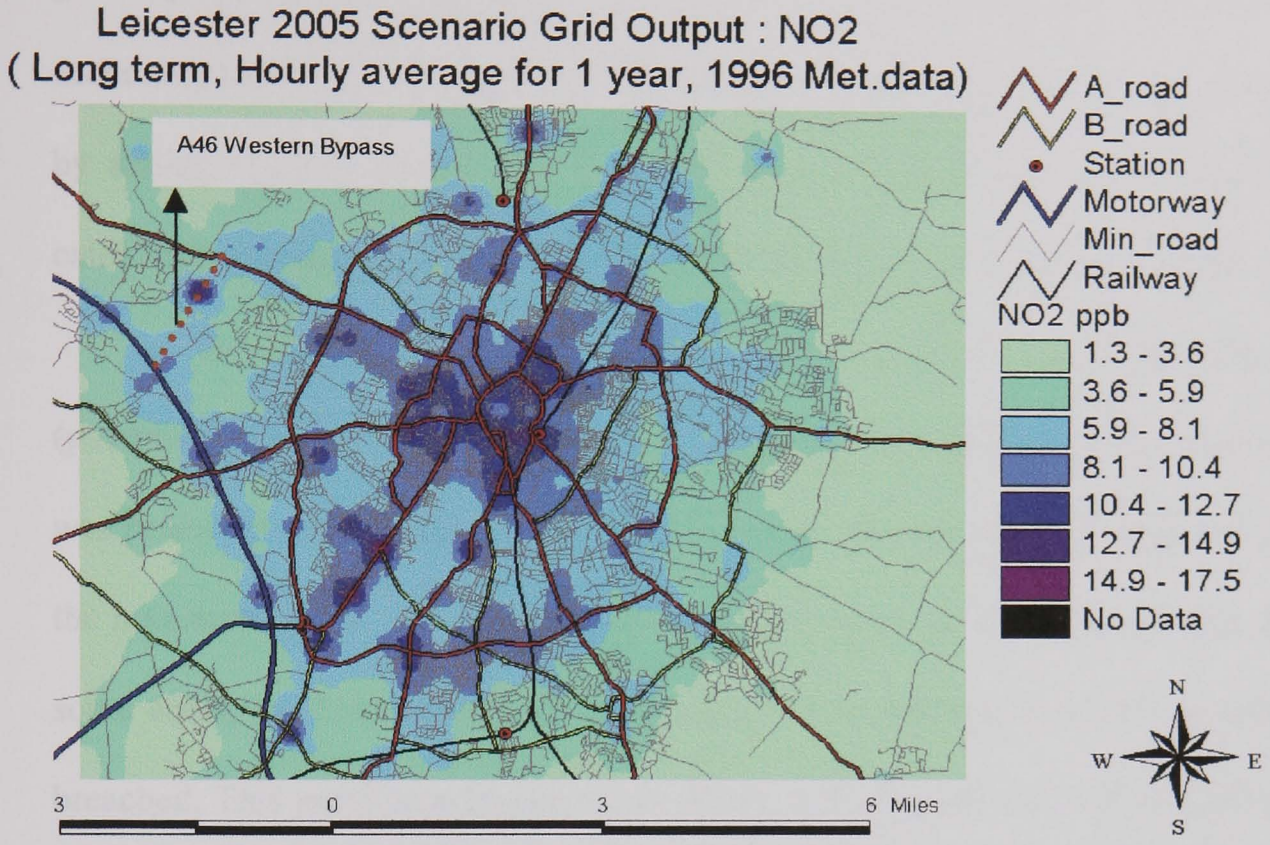
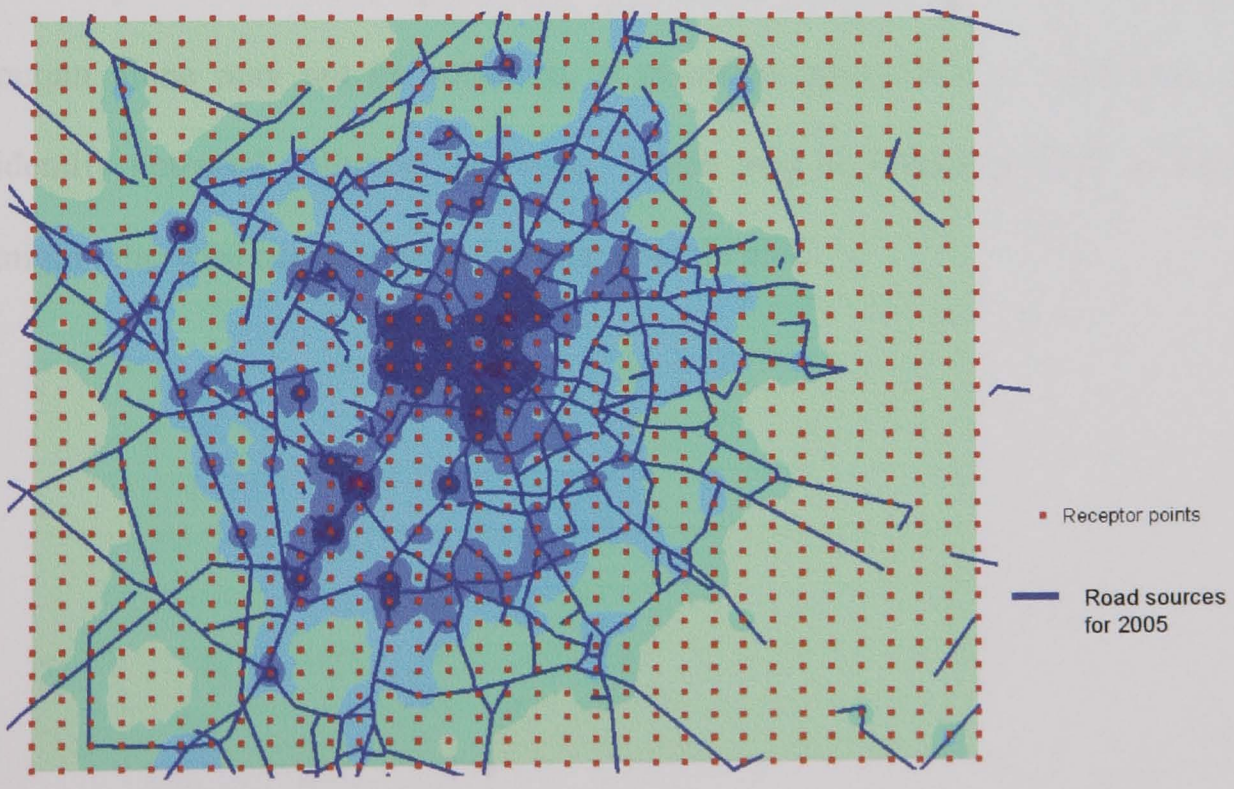


Figure 6.24 Road Sources for 2005 and Receptors in Regular Grid Output



As noted earlier, one of the output options in ADMS_Urban is called "intelligent gridding" (Chapter 3, section 3.2.3). Line sources in "intelligent gridding" are sampled more accurately than that of regular "grid output". "Intelligent gridding" can remove these "blobs" by adding receptor points near the roads so that concentrations all along the roads are calculated and not just at the locations where the regular grid points lie on the roads.

"Intelligent gridding" outputs for 1998 and 2005 across the city centre area (potential high pollution area) are shown in Figure 6.25 and Figure 6.26. The NO_2 pollution was predicted reaching 45.5ppb in 1998 in certain areas as shown in Figure 6.25. However, the maximum values for 2005 are less than 25.5ppb as shown in Figure 6.26. However, for some areas, i.e. busy road junctions, it appears the objective for 2005 is still likely to be breached. This prediction apparently conflicts with the results of regular grid output which no exceendences were found. As "intelligent gridding" takes even longer computational time than the regular grid output (about two to three weeks for a full year meteorological data on a 266HZ Pentium PC, 128MB RAM), it is advisable to choose the output area carefully. When identifying whether there are exceedences in an urban area, regular grid output alone may not be sufficient. It is advantageous to use "intelligent gridding" to identify potential pollution "hot-spots" which may be relatively small in size and which might otherwise not be revealed in a large-scale plot.

Figure 6.25 Leicester City Centre 1998 ADMS_Urban (Intelligent Grid) Output: NO_2

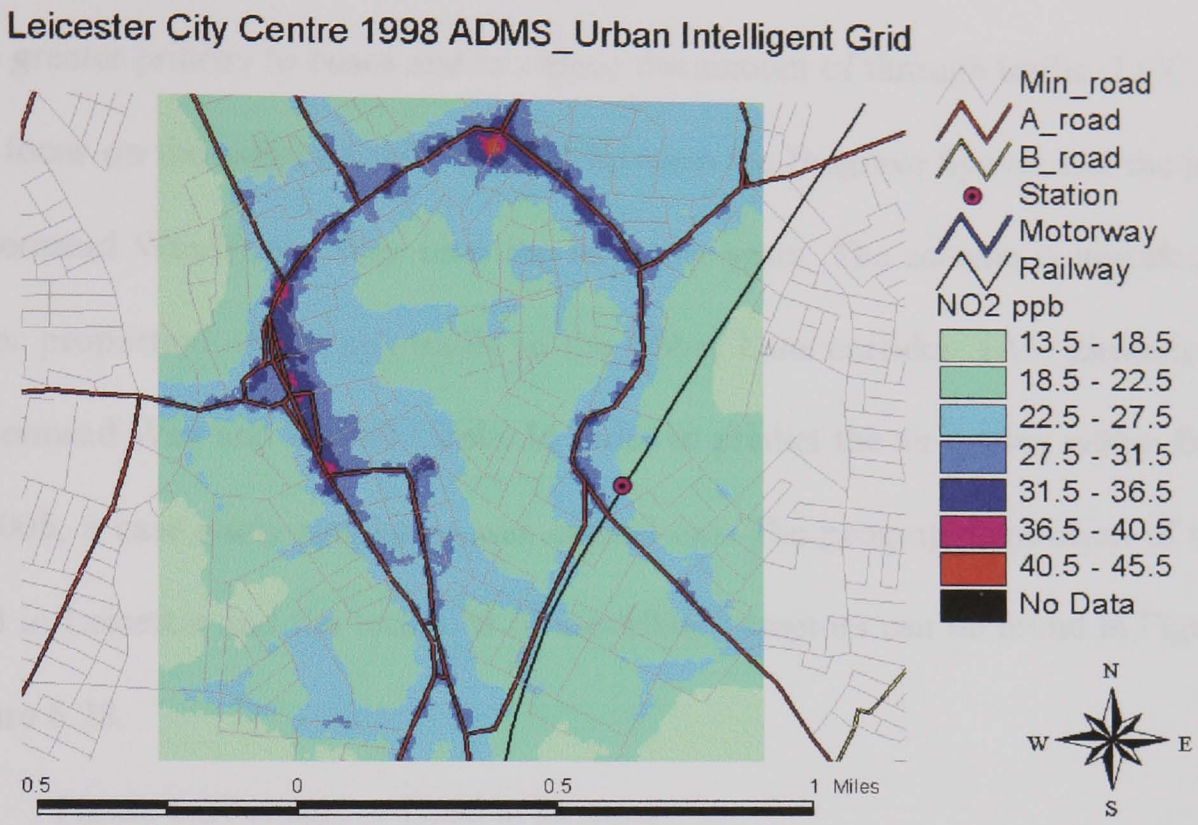
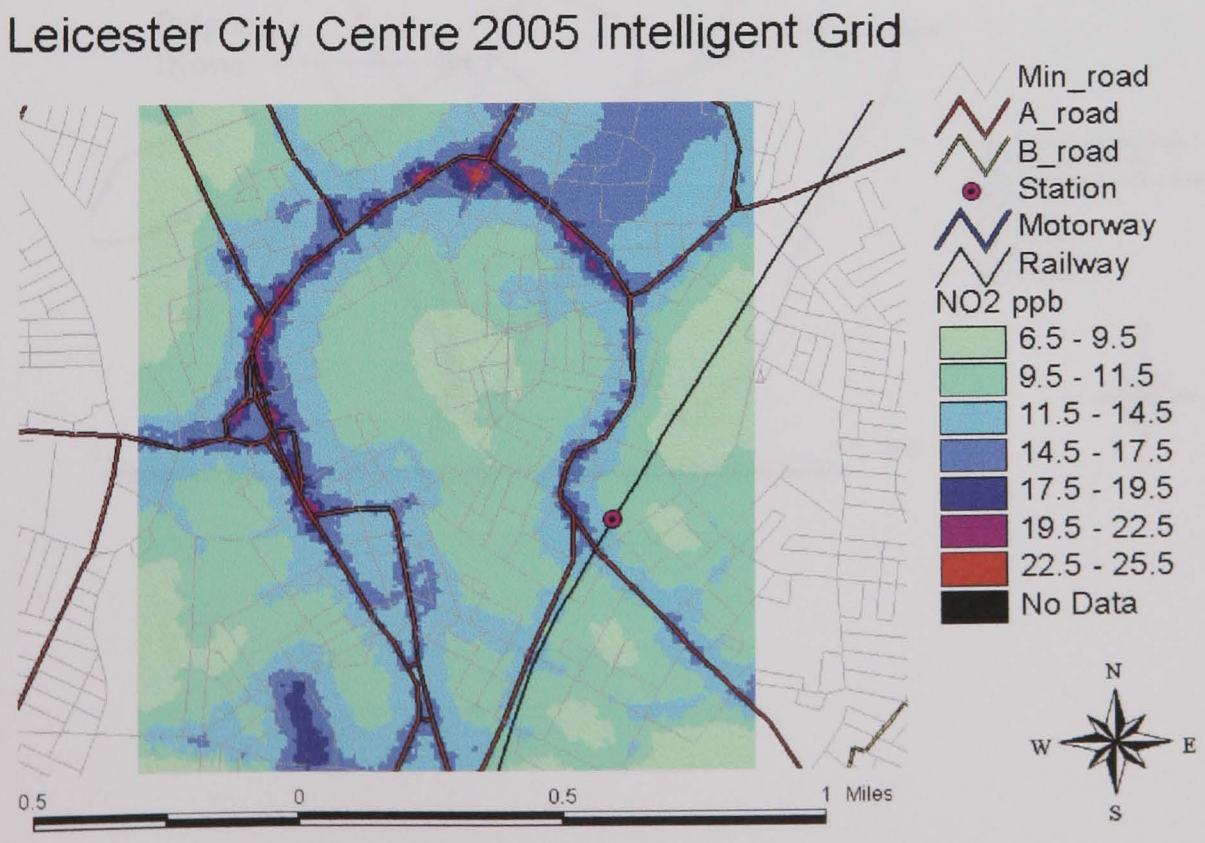


Figure 6.26 Leicester City Centre 2005 ADMS_Urban (Intelligent Grid) Output: NO_2



6.4.5 Belgrave Corridor Scenario Study

Within Leicester's strategic traffic plans, the Belgrave Corridor Project is designed to give greater priority to buses and to reduce the amount of through traffic (LCC, 1999). This will focus on the radial corridor (A607) between the Belgrave flyover and the junction with Watermead Way/Troon Way over the next few years. The scheme is intended to divert a major proportion of through traffic to the Abbey Lane corridor (A6, formerly A5131) via Watermead Way and Redhill Circle. In order to predict the air quality within Belgrave area in 2005, a case study simulation was carried out. The geographic position of the Belgrave road in Leicester and the locations of modelling receptors can be found in Figure 6.27 and Figure 6.28.

Figure 6.27 Belgrave Road in Leicester

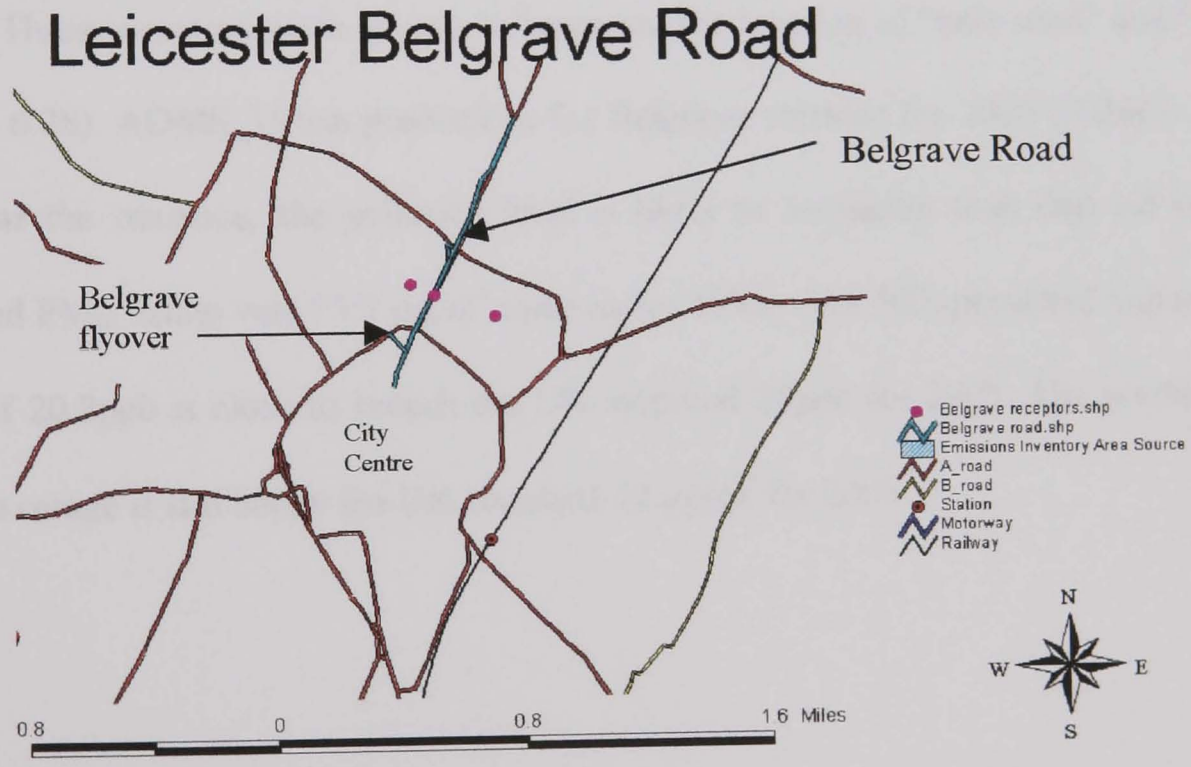
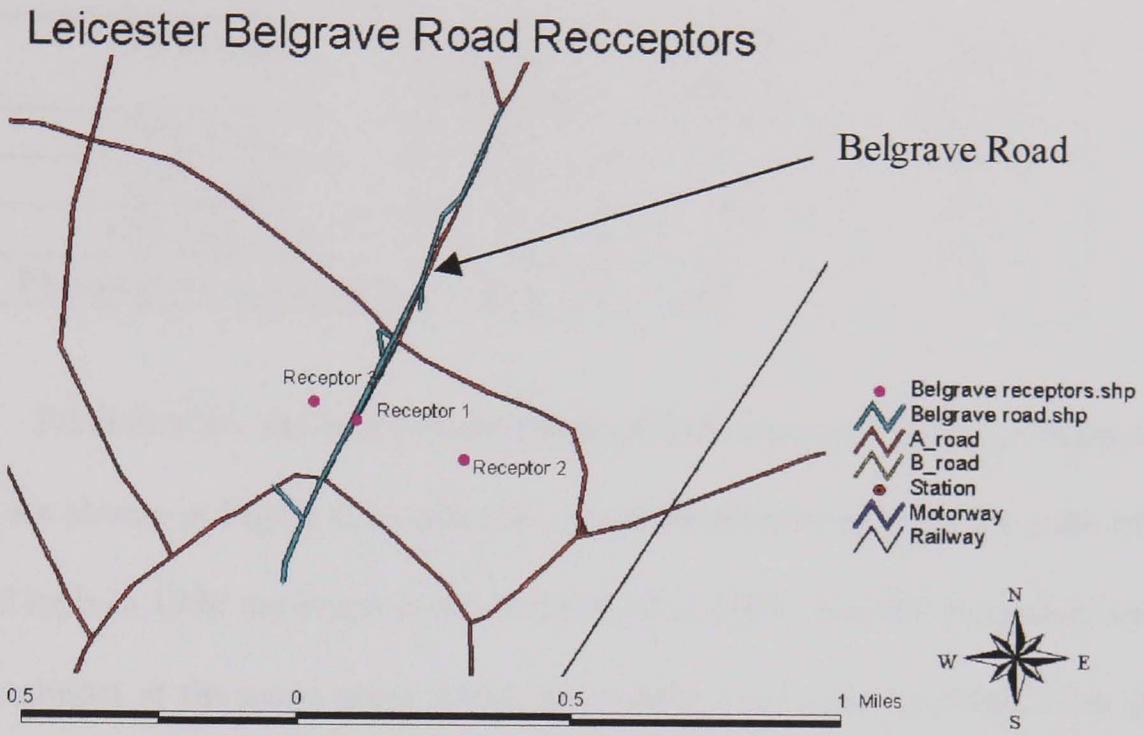


Figure 6.28 Leicester Belgrave Road Receptors



Three receptors were chosen to represent the location of "near road" and "off road" (Figure 6.28). ADMS_Urban predictions for Belgrave corridor for 2005 (Table 6.15) show that near the roadside, the pollution level is likely to be higher than that off roads (the imported PM_{10} values was 13.3 $\mu g/m^3$ same as for 1996). The NO_2 predicted annual average value of 20.2ppb is close to breach the UK standard 21ppb for 2005. The predicted PM_{10} annual average is still below the UK standard 40 $\mu g/m^3$ for 2005.

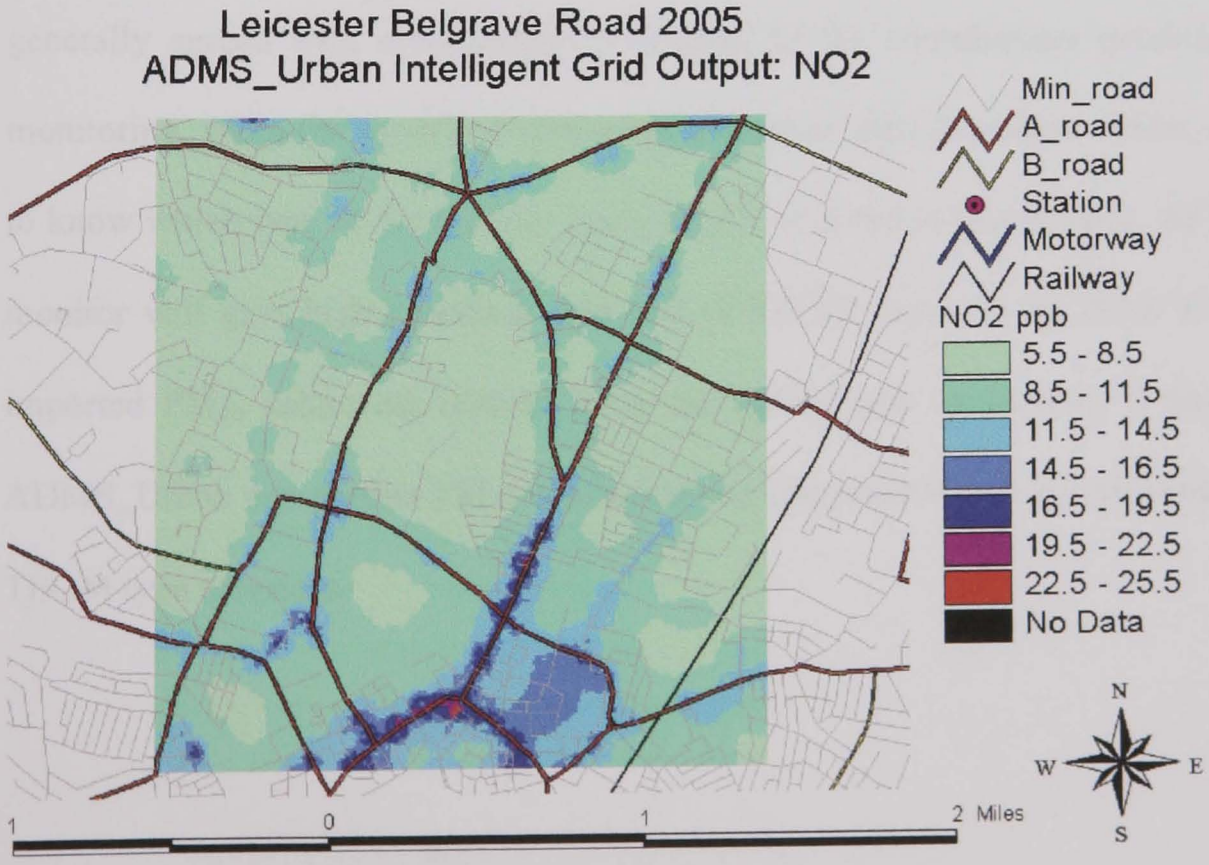
Table 6.15 Belgrave Corridor 2005 Predictions (Annual Average)

Pollutants	Receptor1 Near road	Receptor2 Off road	Receptor3 off road
NO_2 (ppb)	20.2	4.5	6.2
NO_x (ppb)	55.5	6.9	11.2
$PM_{10}(\mu g/m^3)$	3.3	0.4	0.6
$PM_{10}(\mu g/m^3)$ +imported	16.6	13.7	13.9

Prediction for the spatial distribution of NO2 using intelligent gridding for 1998 and 2005 are shown in Figure 6.29 and 6.30. It can be clearly seen that the areas of NO_2 values over 21ppb in 1998 are much lager than that of in 2005. And the maximum values of NO_2 occur almost at the same areas which are mostly busy road junctions. It is still likely to breach the NO_2 objective in those areas in 2005. Those areas therefore should have more air quality control measures to reduce the pollution level.

Figure 6.29 ADMS_Urban 1998 Belgrave Road Prediction: NO_2

Figure 6.30 ADMS_Urban 2005 Belgrave Road Prediction: NO_2



6.5 SUMMARY

The sensitivity test of ADMS_Urban in relation to the location of receptor points at Welford Road suggests that it is important to accurately identify the location of the receptor to be modelled while specifying the model scenarios. Sensitivity tests of input parameters to the output, i.e. vehicle speed, were analysed at Welford Road. It is found that among the input parameters, vehicle speed is one of the important parameters which is most sensitive to the modelled output. Therefore, while preparing the emission database, particular care should be taken to obtain accurate average vehicle speed information. Emission factors used in ADMS_Urban model based on averaged vehicle speed only. As noted in reality, emission factors based on drive cycles can vary greatly from the average speed emission factors. Street Canyon module of ADMS_Urban was tested in Melton Road. If the canyon height is greater than 2m, it is important to specify the street canyon height in the emission database while a roadside receptor is modelled.

The performance of ADMS_Urban to predict the pollution levels of other receptor points besides AUN site was also examined. ADMS_Urban predictions for NO_2 were generally agreed with measurements. Because of the complexities involved with PM_{10} monitoring, when the modelled values are compared with monitored values, it is essential to know which type of the monitor being used. As noted in this chapter, the BAM type of monitor will give higher reading than that of TEOM monitors by about 30%. However, imported PM_{10} values are derived from the TEOM type of monitor. It has been shown ADMS_Urban can predict PM_{10} concentrations comparable with the observed levels from TEOM type monitors.

An emission database for 2005 was constructed. The emission factors used in ADMS_Urban model for 2005 are significantly lower than that for the present time. So despite the expected traffic growth, new clean fuel technologies are expected to have a significant impact reducing overall projected on traffic emissions for 2005.

ADMS_Urban can be successfully used to predict the future air quality in Leicester. A single receptor may not be representative of the future air quality in an urban area. Regular "grid output" and "intelligent gridding" for 1998 and 2005 were therefore examined. "Intelligent gridding" was used to obtain more detailed pollution prediction (higher resolution) over the area of city centre. "Intelligent gridding" outputs for 2005 across the city centre area indicted the maximum predicted values of NO_2 are less than 25.5ppb. However, in some areas, particularly busy roads in the city centre, are found to have exceedences for 2005. Many receptor points have to be used to obtain prediction for the spatial distribution of pollutants. This can be computationally very demanding i.e. run time can be several days or longer for annual predictions. Also gridding techniques may produce artefacts in the spatial plots. These appear as "blobs" of high pollution level (Figure 6.23 and Figure 6.24). Accordingly, spatial plots need to be interpreted with caution.

In addition, a traffic case study at Belgrave corridor was presented. NO_2 predicted annual average is close to breach the standard 21ppb. The predicted PM_{10} annual average is still below the standard 40μg/m^3. ADMS_Urban predicted values for 2005 indicate that near the roadside, the pollution level is likely to breach the standard. This case study provides an indication of usefulness of ADMS_Urban as tool for accessing the impact of local schemes.

CHAPTER 7 CONCLUSIONS, DISCUSSIONS AND FURTHER RESEARCH

7.1 CONCLUSIONS

The primary focus of this study was the application and validation of the ADMS_Urban air dispersion model. The city of Leicester was the setting for all the simulation work. In terms of size, Leicester can be considered to be a fairly typical UK urban environment. The performance of a model simulation is largely dependent on the quality of the input data. This study has examined, in some detail, the creation of the model emission inventory and the air quality monitoring data for model validation purposes. Whilst this study relates to ADMS_Urban as applied in Leicester, the findings and conclusions presented should be representative of any other similar UK urban environment providing that the quality of model input data and general meteorology are comparable.

Leicester has probably the most extensive air quality monitoring network of any UK city outside of London[1]. This has therefore provided a sound basis for validating the performance of ADMS_Urban. The validation of numerical results from the model with available monitoring data was carried out using a variety of data analysis techniques. Overall, it can be concluded that ADMS_Urban could effectively reproduce the main features of air quality within Leicester for the years 1994 to 1998.

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[1] Private communication with LCC.

This study has shown that for the principal gaseous pollutants of concern, e.g. NO_2, ADMS_Urban can produce reasonable results in terms of annual exceedences for the purpose of air quality management (Chapters 5, 6). For the time periods shorter that a year (e.g. month, week), ADMS_urban predictions were generally less reliable. Where the comparison between prediction and measurement was based on time series, the model reproduced the general feature of the measurement, but the instantaneous differences were often large. The study in this thesis demonstrates that it is also possible to obtain acceptable results for the two pollutants that are most difficult to model: PM_{10} Particulates and ozone. The predictions for the PM_{10} Particulates are largely dependant on the amount calculated for import. PM_{10} originating from the emission database were only a small fraction of the predicted total.

The following conclusions can be drawn:

- The emission database was specifically set-up to meet the requirements of ADMS_Urban. It cannot be over-emphasised that dispersion models are only as good as the underlying emission inventories. ADMS_Urban is more sensitive to some model input factors than others. This study has shown that accurate vehicle speeds are one of the most important parameters for predictions of traffic-related pollution levels. As part of this study, guidelines for the creation and application of emissions inventories for air dispersion modelling have been developed as an aid to other ADMS_Urban users.

- Because of the nature of pollution problems prevailing in Leicester, this study has focused on pollutants associated with traffic flows, e.g. NO_2 and PM_{10}. Modelled values against measured values of pollutant concentrations for case studies in Leicester have been undertaken. ADMS_Urban can reliably predict pollution levels of CO, NO_2 and NO_X . The accuracy of model predictions for the annual average NO_2 levels are $\pm$20%

for urban background locations and ±25%~±30% at busy roadside locations. One would expect accuracy to be reduced for shorter time periods.

- In relation to predicting levels of PM_{10} particulates, ADMS_Urban is capable of predicting the PM_{10} from primary sources, but cannot "model" secondary or coarse particulates which are not included in the current emission database. However, import mechanisms incorporated within ADMS_Urban allow additions to be made in relation to both secondary and coarse sources of PM_{10}. It has been shown that by adopting this approach, far more realistic predictions of overall PM_{10} levels can be obtained. Considering the complexity of this issue, ADMS_Urban is capable of producing relatively sound results.

- Sensitivity tests for ADMS_Urban were carried out and model output was found to be particularly sensitive to the location of receptor points, especially where they are close to roads. Therefore, particular care should always be undertaken to accurately locate the position of receptor points.

- Meteorological input data for ADMS_Urban usually consists of historical sequential data from the UK Meteorological Office (or other suppliers). Leicester has an automatic meteorological station, and this local meteorological data was also utilised in this study. This was a relatively new approach and involved developing, in conjunction with CERC, a method for calculating heat flux from local meteorological data. This technique may benefit other model users.

- ADMS_Urban has been found to be an informative tool for predicting air quality in the future. Strategic modelling work, such as assessing future scenarios of air quality for the year 2005, have been carried out. For Leicester it was able to show that for most areas of the City, air quality objectives will be achieved by 2005. However, the use of high resolution spatial outputs (e.g. intelligent grid outputs), showed that there are a number

of relatively localised areas where objectives may be breached. Typically, these are areas immediately adjacent to busy roads. It is of course impossible to validate prediction for future scenarios in advance. Also, exceedences will be sensitive to prevailing meteorological conditions which can vary from year to year. Accordingly, assessments for future scenarios need to be made with caution. The limiting factor is the reliability of future emissions inventories. The uncertainties over future predictions will, at best, be as accurate as "present" predictions. In reality, future predictions are likely to be less reliable than "present" predictions because of all the uncertainties.

- For the practical application of dispersion models for air quality management, the most important quantity is the (predicted) number of exceendences for the year. The accuracy of instantaneous values is of less interest for urban air quality management.

7.2 GUIDELINES AND DISCUSSIONS FOR MODEL USE

The results of this research provide a series of guidelines which can be used by local authorities and other potential ADMS_Urban users to improve model predictions. Requirements concerning model capabilities depend on the particular environmental problem in question and the strategic or regulatory need of the user. The decision makers may need quantitative calculations of certain parameters such as long term average concentration, frequency distributions, maximum concentrations. These calculations have been demonstrated in this study. The use of models for planning purposes is important and the modelling system should therefore be user friendly and give the answers needed for air quality management. Some guidelines formed from this research are summarised below:

- Preparing emission database

  - Information on the operating times of the largest industrial sources, including for instance periods of shutdown, is needed for constructing a good quality emission database.
  - Modelling of roads in ADMS_Urban assumes variation of flow only. Traffic flow data is as a function of time of the day, day of the week and season. If hourly variation data were available, they could be used by the model. It is demonstrable that not all roads exhibit similar diurnal flow variation patterns. Apart from the model run-time considerations, it would be preferable to be able to allow for diurnal variation of flow and speed for each vehicle class, and each road link.
  - Vehicle speeds are assumed to be constant in ADMS_Urban over one road link. During peak flows vehicle speeds will drop and net emissions will therefore be increased. Presently the model only allows for the increase in net emission resulting from increased vehicle flow, not for the attendant decrease in vehicle speeds. While preparing emission database, it will be important to have more accurate vehicle speed values.
  - Estimated values for the emissions of SO_2, NO_2 (as a percentage of NO_x) from traffic and NO_2 from non-road sources significantly affect the predicted values.
  - Because of the limitation of 1500 emission sources in the present version of ADMS_Urban (V1.51), it is advised to use the aggregating tool to group smaller point and line sources into grid sources.

- Meteorological data

Meteorological data is one of the most important input parameters for air dispersion modelling. Standard meteorological data can be obtained from the Meteorological Office. However, if there is no Meteorological office station data available, the use of local meteorological measurements will be necessary. A method of calculating heat flux from

two different height temperature measurements was presented in this study. The knowledge of local wind profile is important to understand the pollution dispersion in the area.

- Design of scenario runs

It is vital to know what can be expected from various model scenarios, i.e. monthly or annual runs, scenarios for specific roads. When modelling NO_2 and NOx, it is important to have remote background data ready, as the GRS scheme in the model will improve the predicted results. When modelling PM_{10}, the secondary and coarse PM_{10} values need to be derived from remote background data. And when comparing the modelled values with monitored values, the instrument used for measurements (i.e. TEOM or BAM) need to be clarified.

As single receptor point may not be representative of the pollution level over an urban area, the grid output and "intelligent gridding" are useful tools to predict the spatial distribution of pollution levels over an urban area. Many receptor points have to be used to obtain prediction for the spatial distribution of pollutants. This can be computationally very demanding i.e. run time can be several days or longer for annual predictions. Also gridding techniques are prone to producing artefacts in the spatial plots. These appear as "blobs" of high pollution level (see section 6.4.4). Accordingly, spatial plots need to be interpreted with caution.

7.3 SUGGESTIONS FOR FURTHER RESEARCH

This study suggests some further investigations are needed. The following points are identified for future study.

Further local scale model development

The model validation exercises described in section 5.3 showed that significant differences exist between the results of the models and monitoring data. Whilst a part of the differences can be attributed to the use of different stability classification schemes and associated dispersion parameters, other elements such as reliability of the meteorological data, the wind profile, and the particular software implementation might also be responsible for some of the differences found.

Future initiatives should be focused on:

- The standard of meteorological input data
- The harmonisation of meteorological pre-processors
- Procedures for model evaluation
- To establish databases for model validations

Study for Effects on humans and ecosystems

To date, little is known about the long-term effects of air pollution on health and ecosystems. Air pollution may not only worsen existing illnesses e.g. asthma, it may also cause it. Evidences for this are emerging and these effects could turn out to be very important (COMEAP, 1998). Further research is recommended on this issue as well as on

other issues such as the loss of life expectancy resulting from the acute effects of air pollution and the effect of air pollution on susceptible groups. Research is also recommended on health outcomes other than deaths and hospital admissions e.g. wheeze. This area is potentially important since more and more people could be affected.

Air quality is one part of environmental impact to be accounted for in planning and decision processes. In this respect an air quality model has to include flexible procedures to identify sensitive parameters and to clarify their functional relationships with emissions and adverse effects of pollution.

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APPENDIX A

BASIC MATHEMATICS DESCRIPTION OF DISPERSION MODELS

A.1 Gaussian Models

The Gaussian plume model is the most common air pollution model. It is based on a simple formula that describes the three-dimensional concentration field generated by a point source under stationary meteorological and emission conditions. The Gaussian plume model is visualised in the equation below, where, for simplicity, the plume is advected towards the positive x-axis. In a general reference system, the Gaussian plume formula is expressed by (Panofsky and Dutton, 1984)

$$c = \frac{Q}{2\pi\sigma_h\sigma_z|\bar{u}|}\exp\left[-\frac{1}{2}\left(\frac{\Delta_{cw}}{\sigma_h}\right)^2\right]\cdot\exp\left[-\frac{1}{2}\left(\frac{z_s+\Delta h-z_r}{\sigma_z}\right)^2\right] \qquad \text{(A-1)}$$

where c (s, r) is the concentration at r = (Xr, Yr, Zr) due to the emissions at s = (Xs, Ys, Zs); Q is the emission rate; σ_h (j_h, d) and σ_z (j_z, d) are the standard deviations (horizontal and vertical) of the plume concentration spatial distribution (often σ_h is referred to as σ_y); j_h and j_z are the horizontal and vertical turbulence states; d is the downwind distance of the receptor from the source, where

$$d = [(r-s)\cdot\bar{u}]/|\bar{u}| \qquad \text{(A-2)}$$

where $\bar{u}$ is the average wind velocity vector at the emission height; Δ_{cw} is the crosswind distance between the receptor and source and Δ_h is the emission plume rise, which is a

function of emission parameter meteorology and downwind distance d. Figure A.1 shows the Gaussian plume rise.

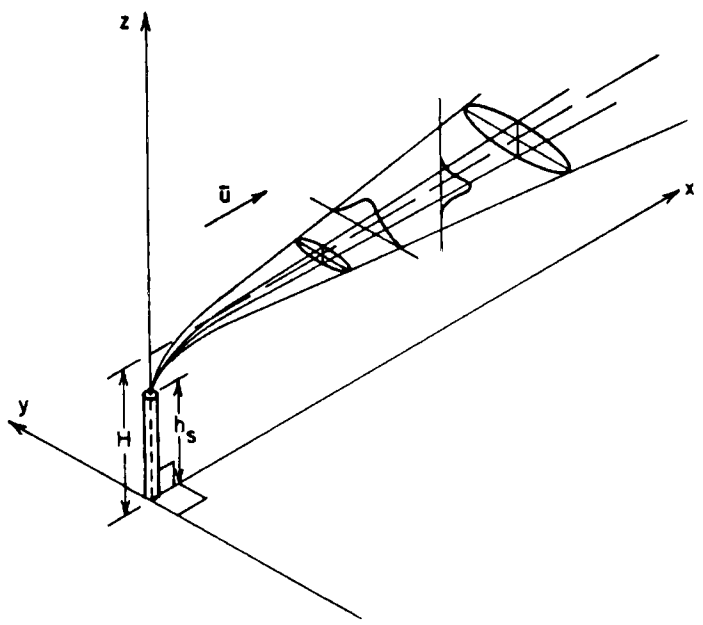

Figure 2.1 Gaussian Plume Rise (source: Dobbins, 1979)

A.2 Eulerian Dispersion Models

The Eulerian approach is based (Lamb, 1980) on the conversion of mass of a single pollutant species of concentration c (x, y, z, t).

$$\frac{\partial c}{\partial t} = -V \cdot \nabla c + D\nabla^2 c + s \qquad \text{(A-3)}$$

Where D is the molecular diffusivity, $\nabla^2 = \partial^2/\partial x^2 + \partial/\partial y^2 + \partial/\partial z^2$ is the Laplacian operator, and ∇ is the gradient operator.

Assume that the velocity V can be represented as the 'sum' of "average" and "fluctuating" components, i.e.

$$V = \bar{u} + u' \tag{A-4}$$

Where $\bar{u}$ represents the portion of the flow that is resolvable using measurements or meteorological models, and u' is the remaining unresolvable component.

Also assume:

$$c = <c> + c' \tag{A-5}$$

Where <> denotes the ensemble (theoretical) mean. which is clarified below. Then, substituting Equations above and taking the ensemble average, the equation below is obtained (Lamb, 1980)

$$\frac{\partial < c >}{\partial t} = -\bar{u} \cdot \nabla < c > -\nabla \cdot < c' u' > + D\nabla^2 < c > + < S > \tag{A-6}$$

In which, according to the ergodic hypothesis, it s assumed that <u> = u and <u'> = 0.

A.3 Lagragian Dispersion Models

Largrangian models provide an alternative method for simulating atmospheric diffusion. They are called Lagrangin because they describe fluid elements that follow the instantaneous flow (Figure A.2).

The fundamental Langrangian equation for atmospheric dispersion of a single pollutant species is (Stull, 1988)

$$< c(r,t) >= \int_{-\infty}^{t} \int p(r,t|r',t')S(r',t')dr'\,dt \qquad \text{(A-7)}$$

Where the integration in space is performed over the entire atmospheric domain; <c(r, t)> is ensemble average concentration at r at time t; S (r', t') is the source term (mass volume^{-1} time^{-1}); and p(r, t|r', t') is the probability density function (volume^{-1}) that an air parcel moves from r' to r at t, where, for any r' and t>t',

$$\int p(r,t \setminus r',t')dr \leq 1 \qquad \text{(A-8)}$$

This expression can be less than one when chemical or deposition phenomena are considered; otherwise, mass conservation always requires the value to be one. For a primary pollutant, S (r', t') is greater than zero only at points r' where the pollutant is released (e.g. the exit points of stacks). For a secondary pollutant, S (r', t') can be nonzero virtually anywhere.

The key parameter in the above equation is the probability density function p, which, for non-reactive pollutants, is a function of only the meteorology (and the type of pollutant when deposition phenomena are considered).

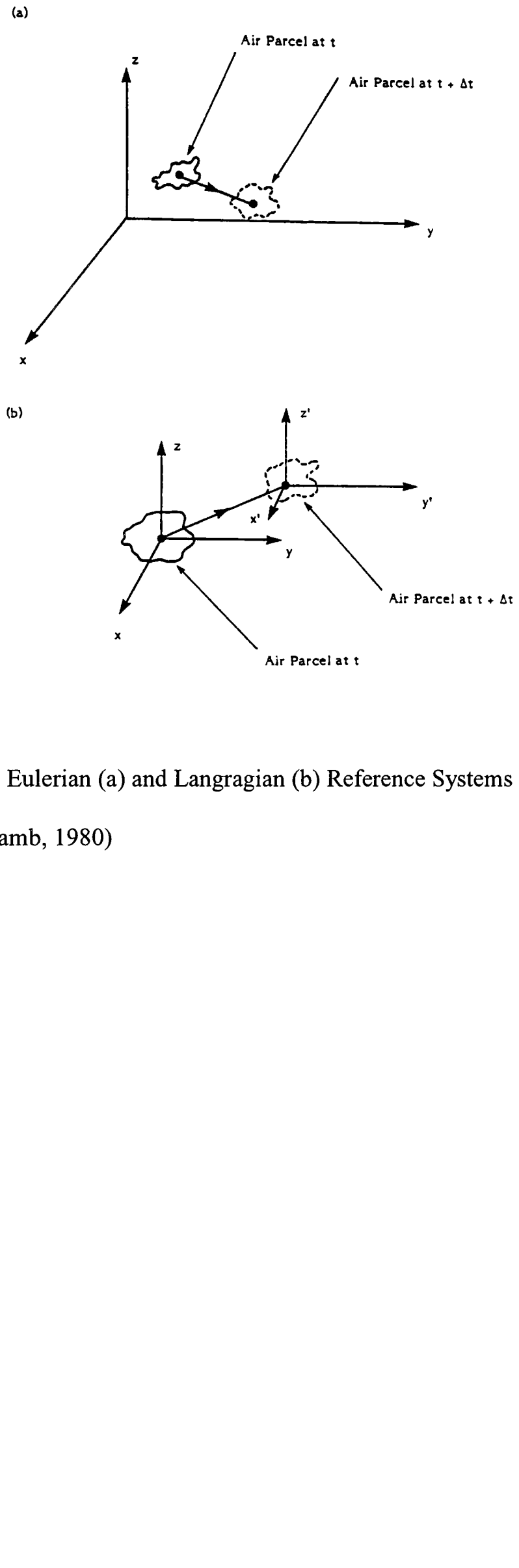

Figure A.2 Eulerian (a) and Langragian (b) Reference Systems for the Atmospheric Motion.

(Source: Lamb, 1980)

Appendix B
Record of ADMS_Urban 1.51 RUNS

Index	Year /month	Start Julian Day	Finish Julian Day	Emission data	Met. Data	Pollutants	Short term (S) or Long term (L)	Receptors	.upl file name
1	1994/June	160	166	Latest emission inventory	Birmingham Elmdon	CO NOx PM10 NO2	S	AUN	xk9406
2	1994/December	359	365	Latest emission inventory	Birmingham Elmdon	CO NOx PM_{10} NO_2	S	AUN	xk9412
3	1995/June	160	166	Latest emission inventory	Birmingham Elmdon	CO NOx PM_{10} NO_2	S	AUN	xk9506
4	1995/November	330	336	Latest emission inventory	Birmingham Elmdon	CO NOx PM_{10} NO_2	S	AUN	xk9511
5	1996/August	180	210	Latest emission inventory	Birmingham Elmdon	CO NOx PM_{10} NO_2	S	AUN	xk9608
6	1996/December	359	366	Latest emission inventory	Birmingham Elmdon	CO NOx PM_{10} NO_2	L	AUN, Grid of city	xk9612, xk9612g
7	1997/Junary	1	6	Latest emission inventory	Birmingham Elmdon	CO NOx PM_{10} NO_2	S	AUN	xk9701

8	1994	1	365	Latest emission inventory	Birmingham Elmdon	CO NOx PM_{10} NO_2	S	AUN	xk94
9	1995	1	365	Latest emission inventory	Birmingham Elmdon	CO NOx PM_{10} NO_2	S	AUN	xk95
10	1996	1	365	Latest emission inventory	Birmingham Elmdon	CO NOx PM_{10} NO_2	S	AUN	xk96
11	1997	1	304	Latest emission inventory	Birmingham Elmdon	CO NOx PM_{10} NO_2	S	AUN	xk97
12	1997	1	365	Latest emission inventory	Leicester Met. Data	CO NOx PM_{10} NO_2	S	AUN	xk97le
13	1998	1	365	Latest emission inventory	Leicester Met. Data	CO NOx PM_{10} NO_2	S	AUN	xk98
14	1994	1	365	Latest emission inventory	Birmingham Elmdon Met.data	SO_2	S	AUN	xk94so2

15	1995	1	365	Latest emission inventory	Birmingham Elmdon Met.data	SO_2	S	AUN	xk95so2
16	1996	1	366	Latest emission inventory	Birmingham Elmdon Met.data	SO_2	S	AUN	xk96so2
17	1997	1	304	Latest emission inventory	Birmingham Elmdon Met.data	SO_2	S	AUN	xk97so2
18	1997	1	365	Latest emission inventory	Leicester Met. Data	SO_2	S	AUN	xk97leso
19	1998	1	365	Latest emission inventory	Leicester Met. Data	SO_2	S	AUN	xk98leso
20	1996	1	366	1998 Road emission data	Birmingham Elmdon Met.data	CO NO_2 NOx PM_{10}	S	AUN	xe98m96
21	1998	1	365	1998 Road emission data	Leicester Met. Data	CO NO_2 NOx PM_{10}	S	AUN	xe98ml98
22	1997	1	304	Latest emission inventory	Birmingham Elmdon Met.data	CO NO_2 NOx PM_{10}	S	8 receptors	Xk97re8

23	1997	1	304	Latest emission inventory	Birmingham Elmdon Met.data	CO NO_2 NOx PM_{10}	S, with O3 background data in UK	AUN	xk97o3b
24	1997	1	304	Latest emission inventory	Birmingham Elmdon Met.data	CO NO_2 NOx PM_{10}	S, with O3 background data in Leicester	AUN	xk97o3l
25	1997	1	304	Latest emission inventory	Birmingham Elmdon Met.data	CO NO_2 NOx PM_{10}	S, with O3 NO2 NOx background data in UK	AUN	xk97o3al
26	1997	1	365	Latest emission inventory	Leicester Met. Data	CO NO_2 NOx PM_{10}	S, with O3 background data in UK	AUN	xk97o3le
27	1994	160	168	Welford road emission	Birmingham Elmdon Met.data	CO NO_2 NOx PM_{10}	S	AUN	Wel3li_2
28	1994	160	168	Welford road emission	Birmingham Elmdon Met.data	CO NO_2 NOx PM_{10}	S	AUN	Wel3link
29	1994	160	168	Welford road emission/Street canyon	Birmingham Elmdon Met.data	CO NO_2 NOx PM_{10}	S	AUN	welrcan4

30	1994	160	168	Welford road emission	Birmingham Elmdon Met.data	CO NO_2 NOx PM_{10}	S	AUN	welroad
31	1994	160	168	Welford road emission/time variation factors	Birmingham Elmdon Met.data	CO NO_2 NOx PM_{10}	S	AUN	weltime
32	1994	160	168	Welford road emission/road width increasing to 20m	Birmingham Elmdon Met.data	CO NO_2 NOx PM_{10}	S	AUN	welwd20
33	1994	160	168	Welford road emission	Birmingham Elmdon Met.data	CO NO_2 NOx PM_{10}	L /grid output	AUN	Wel3gr
34	1996	1	366	1998 emission database	Birmingham Elmdon Met.data	CO NO_2 NOx PM_{10}	S	AUN	x8m96
35	1996	1	366	1998 emission database	Birmingham Elmdon Met.data	CO NO_2 NOx PM_{10}	L/grid output	AUN	xe98m96
36	1998	1	365	2005 Emission database reduced 25%	Leicester Met. Data	CO NO_2 NOx PM_{10}	S/L (Intelligent Grid)	Three receptors Belgrave Area	05belg25

37	1998	1	365	2005 Emission database	Leicester Met. Data	CO NO_2 NOx PM_{10}	S/L	Three receptors	2005belg
38	1996	1	366	1996 Emission database increasing 10%	Birmingham ElmdonMet. Data	CO NO_2 NOx PM_{10}	S	Three receptors	xk96a10
39	1996	1	366	1996 Emission database decreasing 10%	Birmingham Elmdon Met. Data	CO NO_2 NOx PM_{10}	S	Three receptors	xk96d10
40	1996	1	366	2005 Emission database	Birmingham Elmdon Met. Data	CO NO_2 NOx PM_{10}	S/L	AUN	05m96
41	1998	1	365	1998 Emission Database	Leicester Met. Data	NO_2	L	City Centre Area Intelligent Grid	Centre98now
42	1997	1	365	2005 Emission Database	Leicester Met. Data	NO2	L	City Centre Area Intelligent Grid	05cen97

Appendix C

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